

Optimization Theory and Methods

Prof. Xiaoe Ruan

Email: wruanxe@xjtu.edu.cn

[Tel:13279321898](tel:13279321898)

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Chapter 5. Nonlinear Least-Square Method

Gauss-Newton Method

Quasi-Newton update of Gauss-Newton Matrix

Hybrid Algorithm

Decomposed Quasi-Newton Method

Curve fitting problem:

Given data $(z_i, y_i) \in R^{l+1}$ **where** $z_i \in R^l, y_i \in R$.

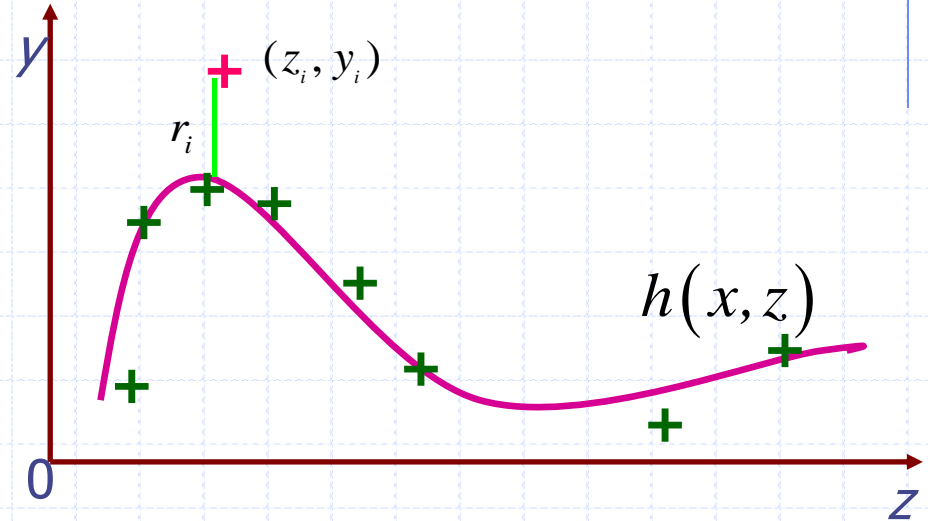
$z_i \neq z_j (i \neq j), i, j = 1, \dots, m$.

Find a nonlinear function

$h(x, z)$ **so that**

**it approximates all of given data
under some criterion**

----- optimal curve fitting.



Least-Square Criterion:

$$\min_{x \in D} f(x) = \sum_{i=1}^m (h(x, z_i) - y_i)^2 = \sum_{i=1}^m (r_i(x))^2$$

$$r(x) = [r_1(x), r_2(x), \dots, r_m(x)]^T \text{ ---residual vector.}$$

1、Gauss-Newton Algorithm

Nonlinear Least-Square Optimization

$$\min_{x \in D} f(x) = \frac{1}{2} \sum_{i=1}^m (r_i(x))^2$$

Denote $r(x) = [r_1(x), r_2(x), \dots, r_m(x)]^T$, $A(x) = (\nabla r_1(x), \dots, \nabla r_m(x))$.

Then $g(x) \triangleq \nabla f(x) = \sum_{i=1}^m \nabla r_i(x) r_i(x) = A(x) r(x)$

$$G(x) \triangleq \nabla^2 f(x) = \underbrace{A(x) A(x)^T}_{M(x)} + \underbrace{\sum_{i=1}^m r_i(x) \nabla^2 r_i(x)}_{S(x)}$$

If $f(x^*) = \min_{x \in D} f(x)$, **then it is possible that** $r_i(x^*) = 0$.

Thus, if $x \in N(x^*)$, **then** $G(x) \approx A(x) A(x)^T = M(x)$.

Let $q_k(d) = f(x^{(k)} + d) \approx f(x^{(k)}) + \nabla f(x^{(k)})^T d + \frac{1}{2} d^T \nabla^2 f(\xi^{(k)}) d$

If $q_k(d^{(k)}) = \min q_k(d)$ **Then**

$$A(x^{(k)})A(x^{(k)})^T d^{(k)} \approx \nabla^2 f(\xi^{(k)})d^{(k)} = -\nabla f(x^{(k)}) = -A(x^{(k)})r(x^{(k)})$$

From $A(x^{(k)})A(x^{(k)})^T d^{(k)} = -g^{(k)} = -A(x^{(k)})r(x^{(k)})$ **yields** $d^{(k)}$.

Gauss-Newton algorithm: $x^{(k+1)} = x^{(k)} + d^{(k)}$.

If $d^{(k)}$ **is descending direction of** $f(x)$,

damped G-N algorithm: $x^{(k+1)} = x^{(k)} + \alpha_k d^{(k)}$.

Features:

(1) $G(x) \approx A(x)A(x)^T \triangleq M(x)$ **only 1-st-order derivative**

(2) $M_k \triangleq M(x^{(k)}) = A(x^{(k)})A(x^{(k)})^T \triangleq A_k A_k^T$ **semi-PD,**

i.e. $d^{(k)}$ **is possibly descending direction.**

(3) Compared with Newton's Method, convergence is influenced.

Th1. Assume that (1) $f(x)$ is 2-nd-order continuously differentiable on open convex set D

(2) There exists $x^* \in D$ s.t. $g(x^*) = A(x^*)r(x^*) = 0$.

(3) $A(x)$ and $G(x)$ satisfying Lipschitz continuous on D

i.e. $\exists \beta, \gamma$ s.t. $\|A(x) - A(y)\| \leq \beta \|x - y\|, \forall x, y \in D,$

and $\|G(x) - G(y)\| \leq \gamma \|x - y\|, \forall x, y \in D,$

(4) $A(x), x \in D$ is full rank and $\|A(x)\| < \sigma, \forall x \in D;$

$\|H(x)\| = \|M(x)^{-1}\| < M, \forall x \in D;$ where $\sigma, M = \text{const.}$

Then, G-N sequence $x^{(k+1)} = x^{(k)} + d^{(k)}$ is meaningful and

$$\|x^{(k+1)} - x^*\| \leq \|H(x^*)S(x^*)\| \|x^{(k)} - x^*\| + O\left(\|x^{(k)} - x^*\|^2\right)$$

Proof: From $A(x), x \in D$ full rank implies $M(x) = A(x)A(x)^\top$ is invertible. Then $d^{(k)}$ is available.

i.e. $x^{(k+1)} = x^{(k)} + d^{(k)}$ is meaningful.

Further $\|A(x) - A(y)\| \leq \beta \|x - y\|, \forall x, y \in D,$

$$\|G(x) - G(y)\| \leq \gamma \|x - y\|, \forall x, y \in D, \quad \|A(x)\| < \sigma, \forall x \in D;$$

Then $\|M(x) - M(y)\|$

$$= \|A(x)A(x)^\top - A(x)A(y)^\top + A(x)A(y)^\top - A(y)A(y)^\top\| \leq 2\sigma\beta \|x - y\|,$$

Therefore $\|H(x) - H(y)\| = \|M(x)^{-1} - M(y)^{-1}\|$

$$= \|M(x)^{-1} [M(y) - M(x)] M(y)^{-1}\| \leq 2M^2 \sigma \beta \|x - y\|,$$

$$\|S(x) - S(y)\| = \|[G(x) - M(x)] - [G(y) - M(y)]\|$$

$$\leq (\gamma + 2\sigma\beta) \|x - y\|, \quad \forall x, y \in D.$$

whilst $0 = g(x^*) = g(x^{(k)}) + G(x^{(k)})(x^* - x^{(k)}) + O_1(\|x^{(k)} - x^*\|^2)$

i.e. $= g(x^{(k)}) + [M(x^{(k)}) + S(x^{(k)})](x^* - x^{(k)}) + O_1(\|x^{(k)} - x^*\|^2)$
 $M(x^{(k)})(x^{(k)} - x^*) = g(x^{(k)}) - S(x^{(k)})(x^{(k)} - x^*) + O_1(\|x^{(k)} - x^*\|^2)$

Therefore $x^{(k+1)} - x^* - (x^{(k+1)} - x^{(k)}) = x^{(k)} - x^*$
 $= M(x^{(k)})^{-1} g(x^{(k)}) - M(x^{(k)})^{-1} S(x^{(k)})(x^{(k)} - x^*) + O_2(\|x^{(k)} - x^*\|^2)$

Then $x^{(k+1)} - x^* = (x^{(k+1)} - x^{(k)}) + M(x^{(k)})^{-1} g(x^{(k)})$
 $- H(x^{(k)}) S(x^{(k)})(x^{(k)} - x^*) + O_2(\|x^{(k)} - x^*\|^2)$

Additionally $x^{(k+1)} - x^{(k)} = d^{(k)} = -M(x^{(k)})^{-1} g^{(k)}$ **Then**

$$x^{(k+1)} - x^* = -H(x^*) S(x^*)(x^{(k)} - x^*) - H(x^{(k)}) [S(x^{(k)}) - S(x^*)](x^{(k)} - x^*)$$

$$- [H(x^{(k)}) - H(x^*)] S(x^*)(x^{(k)} - x^*) + O_2(\|x^{(k)} - x^*\|^2)$$

Thus $\|x^{(k+1)} - x^*\| \leq \|H(x^*) S(x^*)\| \|x^{(k)} - x^*\| + O(\|x^{(k)} - x^*\|^2)$

Discussion: $\|x^{(k+1)} - x^*\| \leq \|H(x^*)S(x^*)\| \|x^{(k)} - x^*\| + O(\|x^{(k)} - x^*\|^2)$

Let $\rho = \|H(x^*)S(x^*)\|$, $O(\|x^{(k)} - x^*\|^2) \leq c \|x^{(k)} - x^*\| \|x^{(k)} - x^*\|$

Then $\|x^{(k+1)} - x^*\| \leq (\rho + c \|x^{(k)} - x^*\|) \|x^{(k)} - x^*\|.$

Thus (1) If $A(x), x \in D$ **is full rank and** $g(x^*) = A(x^*)r(x^*) = 0.$

Then $r(x^*) = 0.$ **i.e.** $S(x^*) = \sum_{i=1}^m r_i(x^*) \nabla^2 r_i(x^*) = 0$ **i.e.** $\rho = 0.$

Then the (damped) G-N algorithm is quadratically convergent.

(2) If $A(x), x \in D$ **is not full rank but** $g(x^*) = A(x^*)r(x^*) = 0.$

then $r(x^*) \neq 0.$ **i.e.** $\rho \neq 0.$ **If** $\rho < 1$, $\|x^{(k)} - x^*\| \ll 1$,

s.t. $\rho + c \|x^{(k)} - x^*\| < 1$ **then G-N algorithm is linearly convergent.**

(3) If $\rho = \|H(x^*)S(x^*)\| \geq 1$ **i.e.** $\|S(x^*)\|$ **is larger**

Then Gauss-Newton algorithm is divergent.

2、Quasi-Newton update of G-N Matrix

$$G(x) \triangleq \nabla^2 f(x) = A(x)A(x)^T + \sum_{i=1}^m r_i(x) \nabla^2 r_i(x)$$

Assume $f(x^*) = \min_x f(x)$, \parallel $M(x)$ \parallel $S(x)$

$$g(x^*) = A(x^*)r(x^*) = 0.$$

If $A(x^*)$ **singular**, **then** $r(x^*) \neq 0$. M_k \parallel C_k

Thus

$$G(x^{(k)}) = M(x^{(k)}) + S(x^{(k)}) \approx M(x^{(k)}) + \sum_{i=1}^m r_i(x^{(k)}) W_i(x^{(k)})$$

where $W_i(x^{(k)}) \approx \nabla^2 r_i(x^{(k)})$ **updated by SR1 formula**

Note $q_k(d) = f(x^{(k)} + d) \approx f(x^{(k)}) + \nabla f(x^{(k)})^T d + \frac{1}{2} d^T \nabla^2 f(\xi^{(k)}) d$

Let $\nabla^2 f(\xi^{(k)}) = M_k + C_k$. **From** $q_k(d^{(k)}) = \min q_k(d)$ **induces** $d^{(k)}$.

-----Brown-Dennis Gauss-Newton matrix SR1 update.

Conclusion:

Brown-Dennis Gauss-Newton SR1 algorithm is convergent.

If $r(x^*) = 0$, B-D G-N algorithm is quadratically convergent.

If the memory is enough, the method is realizable.

Idea: Determine $W_i(x^{(k)}) = \nabla^2 r_i(x^{(k)})$ by update formula

Requirement : Quasi-N Eq. $B_{k+1}\delta^{(k)} = y^{(k)}$. $\delta^{(k)} = x^{(k+1)} - x^{(k)}$

As
$$y^{(k)} \triangleq \nabla f(x^{(k+1)}) - \nabla f(x^{(k)}) = \nabla^2 f(\bar{x}^{(k)})(x^{(k+1)} - x^{(k)})$$
$$= G(\bar{x}^{(k)})(x^{(k+1)} - x^{(k)}) = [M(\bar{x}^{(k)}) + S(\bar{x}^{(k)})](x^{(k+1)} - x^{(k)})$$

Thus
$$S(\bar{x}^{(k)})(x^{(k+1)} - x^{(k)}) = y^{(k)} - M(\bar{x}^{(k)})(x^{(k+1)} - x^{(k)}). \quad \text{i.e.}$$

quasi-N Eq. $C_{k+1}\delta^{(k)} = \gamma^{(k)}$ is satisfied. $\gamma^{(k)} = y^{(k)} - M(\bar{x}^{(k)})(x^{(k+1)} - x^{(k)})$.

Difference of $M_k, \gamma^{(k)}$ produce different updates.

Generalization 1:

Brown-Dennis Gauss-Newton SR2 update:

Let $M\left(\bar{x}^{(k)}\right) = A\left(x^{(k+1)}\right) A\left(x^{(k+1)}\right)^{\top} \triangleq M_k$

$$\gamma^{(k)} = g^{(k+1)} - g^{(k)} - M_k \delta^{(k)}.$$

$$S\left(\bar{x}^{(k)}\right) = C_{k+1} = C_k + \Delta C_k \quad \text{updated by SR2 formula}$$

Generalization 2:

Betts Gauss-Newton update:

$$M_k = A\left(x^{(k)}\right) A\left(x^{(k)}\right)^{\top}, \quad \gamma^{(k)} = g^{(k+1)} - g^{(k)} - M_k \delta^{(k)}.$$

$$S\left(\bar{x}^{(k)}\right) = C_{k+1} = C_k + \Delta C_k \quad \text{updated by quasi-N SR2 formula}$$

Gen.3: Bartholomew-Biggs, Dennis-Gay-Welsch Gauss-

Newton update

$$M_k = A\left(x^{(k+1)}\right)A\left(x^{(k+1)}\right)^T, \quad \gamma^{(k)} = \left[A_{k+1} - A_k\right]r^{(k+1)}, \quad \eta^{(k)} = \gamma^{(k)} - C_k\delta^{(k)},$$
$$S\left(\bar{x}^{(k)}\right) = C_{k+1} = C_k + \frac{y^{(k)}\eta^{(k)T} + \eta^{(k)}y^{(k)T}}{\delta^{(k)T}y^{(k)}} - \frac{\delta^{(k)T}\eta^{(k)}}{\left[\delta^{(k)T}y^{(k)}\right]^2}y^{(k)}y^{(k)T}$$

Gen.4: Gill-Murray Gauss-Newton update

$$M_k = A\left(x^{(k+1)}\right)A\left(x^{(k+1)}\right)^T, \quad \gamma^{(k)} = g^{(k+1)} - g^{(k)} - M_k\delta^{(k)}, \quad W_k = A_{k+1}A_{k+1}^T + C_k,$$
$$S\left(\bar{x}^{(k)}\right) = C_{k+1} = C_k + \frac{y^{(k)}y^{(k)T}}{\delta^{(k)T}y^{(k)}} - \frac{W_k\delta^{(k)}\delta^{(k)T}W_k}{\delta^{(k)T}W_k\delta^{(k)}}$$

Conclusion:

Gill-Murray Gauss-Newton update-based sequence is locally superlinearly convergent.

Remarks:

(1) $S(\bar{x}^{(k)}) = C_{k+1}$ may be inappropriate, Efficiency ??

May employ tuning factor such as $C_{k+1} = \tau_k C_k + \Delta C_k$

(2) C_k May be non-PD. Thus $G_k = M_k + C_k$ may be non-PD.

Hence $d^{(k)}$ may be non-descending direction.

Possible ways:

Trust-region technique or decomposed quasi-Newton method.

(3) At the beginning iterations, adopt Gauss-Newton method.

Then switch to Gauss-Newton quasi-N update-based method.

(4) Solve Eq. of searching direction by proper manner.

3. Hybrid Algorithm

Combine Gauss-Newton algorithm with some unconstrained optimization method and automatically switch to a proper method.-----Switching method.

Powell's hybrid algorithm

Rotate Gauss-Newton direction to negative gradient for searching direction.

Gauss-Newton direction:

Let $q_k(d) = f(x^{(k)} + d) = f(x^{(k)}) + \nabla f(x^{(k)})^T d + \frac{1}{2} d^T \nabla^2 f(\xi^{(k)}) d$

If $q_k(d^{(k)}) = \min q_k(d)$ **Then**

$$A(x^{(k)}) A(x^{(k)})^T d^{(k)} = -A(x^{(k)}) r(x^{(k)}) \quad \text{achieving} \quad d^{(k)}.$$

Powell's Hybrid Algorithm

From $\min \sum_{i=1}^m \left[\frac{r(x^{(k)}) - \alpha \nabla r(x^{(k)})^T \frac{g^{(k)}}{\|g^{(k)}\|}}{\|g^{(k)}\|^3} \right]^2$

get $\alpha_k = \frac{\|g^{(k)}\|^3}{g^{(k)T} A_k A_k^T g^{(k)}}$

$\alpha_k \geq \Delta_k$

Yes

$d^{(k)} = -\Delta_k \frac{g^{(k)}}{\|g^{(k)}\|}$

No

$d_{CP}^{(k)} = -\alpha_k \frac{g^{(k)}}{\|g^{(k)}\|}$

From $\|d_{CP}^{(k)} + \lambda (d_{GN}^{(k)} - d_{CP}^{(k)})\| = \Delta_k$ **get** λ_k

$d^{(k)} = d_{CP}^{(k)} + \lambda_k (d_{GN}^{(k)} - d_{CP}^{(k)})$

solve $d_{GN}^{(k)}$ **from** $A_k A_k^T d^{(k)} = -A_k r^{(k)}$

No

$\|d_{GN}^{(k)}\| \leq \Delta_k$

Yes

$d^{(k)} = d_{GN}^{(k)}$

Construction of $d^{(k)}$ for $\alpha_k < \Delta_k$

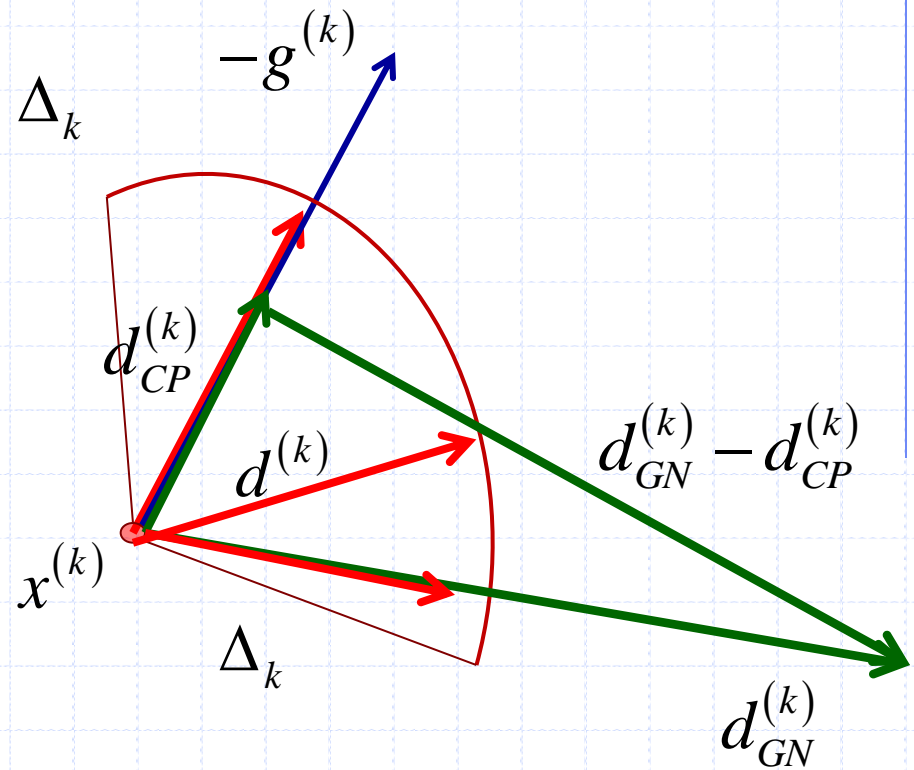
Then

If $f\left(x^{(k)} + d^{(k)}\right) < f\left(x^{(k)}\right)$

Let $x^{(k+1)} = x^{(k)} + d^{(k)}.$

Otherwise,

tuning $\Delta_k.$



Powell proved that the hybrid algorithm is convergent but only modification of Gauss-Newton method with no much improvement of convergence rate.

Comparison:

Gauss-Newton Algorithm	BFGS quasi-N Algorithm
Utilizing 1-st-order derivative to estimate 2-nd derivative according to structure of LS problem.	Utilizing 1-st-order derivative to estimate 2-nd derivative of objective fcn but needs multi-update.
Quadratic convergent for zero-residual pbm.	Superlinear convergent for zero-residual pbm.
Linearly convergent for smaller-residual pbm and faster near minimizer.	Superlinearly convergent for smaller-residual pbm and slower near minimizer.
Not or linearly convergent for larger-residual pbm.	Superlinearly convergent for larger-residual pbm.

Al-Baali-Fletcher Hybrid Algorithm

Combine Gauss-Newton M with BFGS quasi-N M for searching direction.

BFGS update

$$B_k = BFGS \left(B_{k-1}, \delta^{(k-1)}, y^{(k-1)} \right)$$
$$= B_{k-1} + \frac{y^{(k-1)} y^{(k-1)T}}{y^{(k-1)T} \delta^{(k-1)}} - \frac{B_{k-1} \delta^{(k-1)} \delta^{(k-1)T} B_{k-1}^T}{\delta^{(k-1)T} B_{k-1} \delta^{(k-1)}}$$

Switching criterion of Al-Baali-Fletcher hybrid algorithm:

Let

$$\Delta(B, \delta, y) = \left(\frac{y^T B^{-1} y}{\delta^T y} \right)^2 - \frac{2\delta^T y}{\delta^T B \delta} + 1$$

----approximation degree of B to $\nabla^2 f(x)$

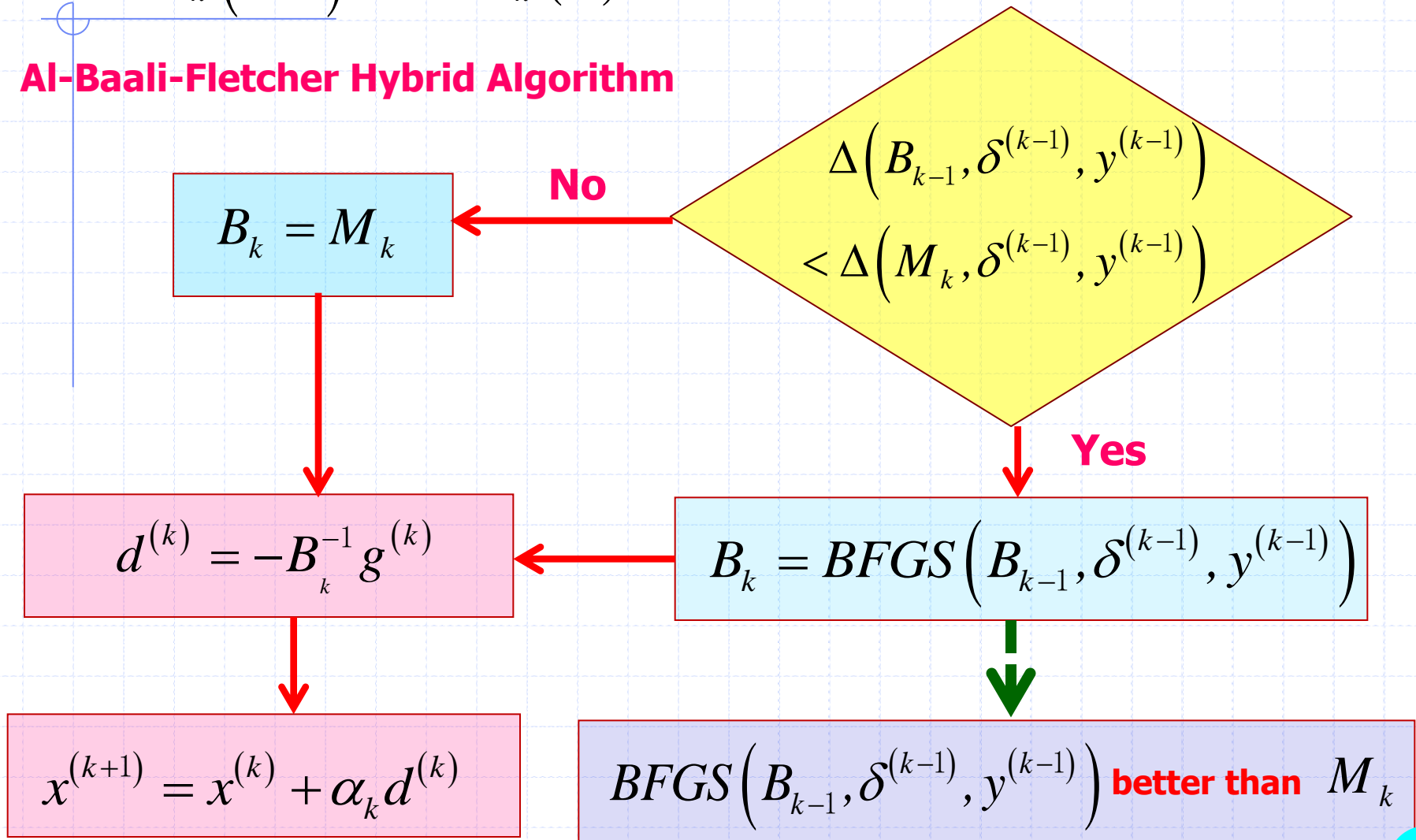
Switching criterion:

$$\Delta \left(B_{k-1}, \delta^{(k-1)}, y^{(k-1)} \right) < \Delta \left(M_k, \delta^{(k-1)}, y^{(k-1)} \right)$$

Let $q_k(d) = f(x^{(k)} + d) = f(x^{(k)}) + \nabla f(x^{(k)})^T d + \frac{1}{2} d^T B_k d,$

From $q_k(d^{(k)}) = \min q_k(d)$ **yields** $d^{(k)} = -B_k^{-1} g^{(k)}.$

Al-Baali-Fletcher Hybrid Algorithm



Remarks:

(1) ABF hybrid algorithm guarantees B_k PD. Thus $d^{(k)}$ is descending direction. α_k determined by simple method.

(2) AI-Baali-Fletcher hybrid algorithm is effective.

(3) For smaller-residual pbm, G-N algorithm is quadratically convergent, whilst for larger-residual pbm, BFGS algorithm is superlinearly convergent. Therefore,

ABF hybrid algorithm does not guarantee superlinear convergence.

Fletcher-Xu switching criterion:
$$\frac{f(x^{(k-1)}) - f(x^{(k)})}{f(x^{(k-1)})} < \rho, \quad \rho \in (0, 1).$$

Recommendation: $\rho = 0.2$. Then

ABF hybrid algorithm eventually switches to BFGS algorithm which means Fletcher-Xu algorithm is superlinearly convergent.

4、Decomposed Quasi-Newton Algorithm

$$G(x) \triangleq \nabla^2 f(x) = \overbrace{A(x)A(x)^T}^{M(x)} + \overbrace{\sum_{i=1}^m r_i(x) \nabla^2 r_i(x)}^{S(x)}$$

$$G(x^{(k)}) = M(x^{(k)}) + S(x^{(k)}) = \overbrace{M(x^{(k)})}^{A_k A_k^T} + \underbrace{\sum_{i=1}^m r_i(x^{(k)}) \nabla^2 r_i(x^{(k)})}_{L_k L_k^T + L_k A_k^T + A_k L_k^T}$$

Let $q_k(d) = f(x^{(k)} + d)$

$$= f(x^{(k)}) + \nabla f(x^{(k)})^T d + \frac{1}{2} d^T B_k d,$$

$$B_k = A_k A_k^T + L_k L_k^T + L_k A_k^T + A_k L_k^T = (A_k + L_k)(A_k + L_k)^T.$$

From $q_k(d^{(k)}) = \min q_k(d)$ **reaches** $d^{(k)}$ **s.t.** $B_k d^{(k)} = -A_k^T r^{(k)}$

Decomposed quasi-Newton algorithm: $x^{(k+1)} = x^{(k)} + d^{(k)}.$

Discussion:

(1) If row rank of $A_k + L_k$ is full, then $B_k = (A_k + L_k)(A_k + L_k)^T$ PD.

Thus $d^{(k)}$ is descending direction.

(2) Quasi-N Eq. $B_k \delta^{(k)} = (A_k + L_k)(A_k + L_k)^T \delta^{(k)} = y^{(k)}$.

(3) If $\delta^{(k)T} y^{(k)} \neq 0$, then $B_k \delta^{(k)} = y^{(k)}$ has solution.

Hence

$$(A_k + L_k)(A_k + L_k)^T \delta^{(k)} = y^{(k)} \Rightarrow \begin{cases} (A_k + L_k)h = y^{(k)} \\ (A_k + L_k)^T \delta^{(k)} = h \\ h^T h = \delta^{(k)T} y^{(k)} \end{cases}$$

Update L_{k+1} by construction of h

Denote $R_{k+1} = A_{k+1} + L_{k+1}$, $V_k = A_{k+1} + L_k$, $W_k = V_k V_k^T$.

If W_k **nonsingular.**

Let $h = aV_k^T \delta^{(k)} + bV_k^T W_k^{-1} y^{(k)}$,

From $(A_{k+1} + L_{k+1})h = y^{(k)}$ **yields** $A_{k+1} + L_{k+1} = X_0 + \bar{Y}$.

$$X_0 = a \frac{y^{(k)} \delta^{(k)T} V_k}{\delta^{(k)T} y^{(k)}} + b \frac{y^{(k)} y^{(k)T} W_k^{-1} V_k}{\delta^{(k)T} y^{(k)}},$$

$$\bar{Y} = cV_k \left[I - \frac{V_k^T \delta^{(k)} \delta^{(k)T} V_k}{\delta^{(k)T} W_k \delta^{(k)}} \right] + d \left[I - \frac{y^{(k)} \delta^{(k)T}}{\delta^{(k)T} y^{(k)}} \right] V_k.$$

where a, b, c, d **to be determined satisfying**

$$a^2 \delta^{(k)T} W_k \delta^{(k)} + 2ab \delta^{(k)T} y^{(k)} + b^2 y^{(k)T} W_k^{-1} y^{(k)} = \delta^{(k)T} y^{(k)},$$

$$ad \delta^{(k)T} W_k \delta^{(k)} - bc \delta^{(k)T} y^{(k)} = 0, \quad c + d = 1.$$

Update of L_{k+1}

$$L_{k+1} = L_k + (a - d) \frac{y^{(k)} \delta^{(k)T} V_k}{\delta^{(k)T} y^{(k)}} + b \frac{y^{(k)} y^{(k)T} W_k^{-1} V_k}{\delta^{(k)T} y^{(k)}} - c \frac{W_k \delta^{(k)} \delta^{(k)T} V_k}{\delta^{(k)T} W_k \delta^{(k)}}$$

Substituting into $B_{k+1} = (A_{k+1} + L_{k+1})(A_{k+1} + L_{k+1})^T$ **achieves** B_{k+1}

Difference of update formula depends on choices of a, b, c, d

Feature: **Update invariance under linear transformation.**

Conclusion: **For** $f(x) = \frac{1}{2} \sum_{i=1}^m r_i^2(x),$

when $A(x), G(x)$ **satisfy some conditions**

Decomposed quasi-Newton algorithm is linearly convergent.

THANK YOU FOR ATTENDING

