

$$\vec{x} \in E^n, \nabla^2 f(\vec{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \dots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

$$\operatorname{tr} A = \sum_{i=1}^n \lambda_i, \det A = \prod_{i=1}^n \lambda_i$$

for  $n \times n$  matrix  $A$ .

Sylvester's Criterion - real, symmetric  $A$  positive definite  $\Leftrightarrow$  All principal minors of  $A$  are positive.

$\Leftrightarrow$  all upper  $K \times K$  corners of  $A$  are minors w/ positive determinants.  
Also  $[A_{11}] < 0 \Rightarrow A$  not positive definite.

min/max function  $f: E^n \rightarrow E$  on  $K \subseteq E^n$ ,  $K = E^n$  (unconstrained),  $K \neq E^n$  (constrained)

Existence

0th order sufficient conditions for rel min

Soln for: minimize  $f$  subject to:  $h_i = 0, i=1, \dots, m; g_j \leq 0, j=1, \dots, r$

Sufficient condition for solution -  $f$ : continuous,  $K$  compact (closed and bounded)  $\Rightarrow f$  has min in  $K$ .

$\hookrightarrow h_i, g_j$  continuous  $\Rightarrow$  set satisfying  $h_i = 0, g_j \leq 0$  closed,  $\exists R > 0: K \subseteq B_R(0) = \{\vec{x} \in E^n : \|\vec{x}\| < R\} \Rightarrow K$  bounded

Unconstrained -  $\exists \vec{x}_0, \exists R > 0: \forall \vec{x} \quad \|\vec{x}\| > R \Rightarrow f(\vec{x}_0) < f(\vec{x}) \Rightarrow f$  has min.

$f \in C^1$  [continuously differentiable] on  $K$ ,  $\vec{x}$  relative min of  $f$  in  $K \Rightarrow \forall \vec{j}$  feasible directions,  $\nabla f(\vec{x}) \cdot \vec{j} \geq 0$

rel min -  $\exists \vec{x}, \exists \epsilon > 0 \quad \forall \vec{x}' : \|\vec{x} - \vec{x}'\| < \epsilon \Rightarrow f(\vec{x}') > f(\vec{x}), \vec{j}$  feasible direction at  $\vec{x} \quad \exists \alpha > 0 \quad \forall 0 < \alpha < \epsilon: \vec{x} + \alpha \vec{j} \in K$

for specific  $\vec{x}$   $\vec{x}$  interior in  $K \Rightarrow \forall \vec{j} \quad \nabla f(\vec{x}) \cdot \vec{j} \geq 0 \Rightarrow \nabla f(\vec{x}) = \vec{0}$ .

$f \in C^2$  on  $K$ ,  $\vec{x}$  rel min of  $f \Rightarrow \forall \vec{j}$  feasible directions  $\nabla f(\vec{x}) \cdot \vec{j} \geq 0$  or  $\nabla f(\vec{x}) \cdot \vec{j} = 0 \wedge \vec{j}^T \nabla^2 f(\vec{x}) \vec{j} \geq 0$

$\hookrightarrow \vec{j}^T \nabla^2 f(\vec{x}) \vec{j} \geq 0 \Leftrightarrow$  eigenvalues all  $\geq 0$  (positive semidefinite)

$f \in C^2$  on  $K$ ,  $\vec{x}$  interior point of  $K$ ,  $\nabla f(\vec{x}) = \vec{0}, \nabla^2 f(\vec{x}) > 0$  [ $\nabla^2 f(\vec{x})$  positive definite]  $\Rightarrow \vec{x}$  strict rel min.

$C \subseteq E^n$  convex if  $\forall \vec{x}, \vec{y} \in C, \forall 0 < \alpha < 1: \alpha \vec{x} + (1-\alpha)\vec{y} \in C, C, D$  convex,  $\beta \in \mathbb{R} \Rightarrow \beta C, C + D, \{x\}, \emptyset$ ,  $C \cap D$  convex.

Convex sets  $f$  convex on convex set  $K$  if  $\forall x, y \in K, \forall 0 \leq \alpha \leq 1 \quad f(\alpha y + (1-\alpha)x) \leq \alpha f(y) + (1-\alpha)f(x)$

$\hookrightarrow f_1, f_2$  convex,  $\alpha \geq 0 \Rightarrow f_1 + f_2, \alpha f_1, \{x \in K : f(x) \leq a\}$  convex.

$\hookrightarrow f \in C^1, K$  convex,  $f$  convex  $\Leftrightarrow \forall \vec{x}, \vec{y} \in K, f(\vec{y}) \geq f(\vec{x}) + \nabla f(\vec{x})(\vec{y} - \vec{x})$

$\hookrightarrow f \in C^2, K$  convex  $f$  convex  $\Leftrightarrow \forall \vec{x} \in K, \nabla^2 f(\vec{x})$  positive semidefinite.

$\hookrightarrow f$  convex, Epigraph  $\{(r, \vec{x}) | r \geq f(\vec{x})\}$  is convex, too.

$f$  convex on convex set  $K \Rightarrow$  any local min is a global min.

FEC<sup>1</sup>, convex on convex set  $K \quad \exists \vec{x}$  s.t.  $\nabla f(\vec{x})(\vec{y} - \vec{x}) \geq 0 \quad \forall \vec{y} \in K \Rightarrow \vec{x}$  global min of  $f$  on  $K$ .

Hyperplane -  $(n-1)$  deg subspace,  $\{\vec{x} \in E^n : \vec{a}^T \vec{x} = c\} \quad \vec{a} \neq \vec{0}, c \in \mathbb{R}$ . For Hyperplane  $H$ ,  $H_+ = \{\vec{x} \in E^n : \vec{a}^T \vec{x} > c\}$  upper half space

$B, C$  convex, no interior intersection, then there is a hyperplane separating them. If only intersect at boundary,  $\exists H$

and  $B \cap C \subseteq H$ ,  $B \subseteq H_+$ ,  $C \subseteq H_-$ . i.e.,  $H = \{\vec{x} \in E^n : \vec{a}^T \vec{x} = c\} \quad \forall b \in B, \vec{c} \in C: \vec{a}^T \vec{b} > c, \vec{a}^T \vec{c} \leq c$ .

$f$  convex on  $K$  convex,  $\vec{x}$  min of  $f \Rightarrow \exists \vec{x} \neq \vec{0}$  s.t.  $\vec{x}$  satisfies: (1)  $\min f(x) + \vec{a}^T \vec{x}, \vec{x} \in E^n$  (2)  $\max \vec{a}^T \vec{x}, \vec{x} \in K$ .

Convex polytope  $\{\vec{x} \in E^n : \vec{a}_1 \vec{x} \leq c_1, \dots, \vec{a}_n \vec{x} \leq c_n\}$ , for  $\vec{a}_i \in E^n, c_i \in \mathbb{R}$ . Polyhedron = bounded convex polytope.

Algorithms -  $A: X \rightarrow P(X) = \{\text{output you could get by running some program w/ procedure you have in mind}\} \rightarrow$  point-set

Segments:  $x_0, x_1 \in A(x_0), x_2 \in A(x_1), \dots, x_n \in A(x_n)$ . Goal Set -  $\Gamma \subseteq X$  (usually  $\{\min f\}$ )

Descent Function -  $Z: X \rightarrow \mathbb{R}$  s.t. 1)  $\forall k \in \mathbb{N}, x_k \in A(x_k) \Rightarrow Z(x_k) > Z(x_{k+1})$  2)  $\forall k \in \mathbb{N}, x_{k+1} \in A(x_k) \Rightarrow Z(x_k) > Z(x_{k+1})$

$A: X \rightarrow Y$  closed at  $x \in X$  if:  $x_k \rightarrow x, x_k \in X, y_k \rightarrow y, y_k \in A(x_k) \Rightarrow y \in A(x)$ , IP: A point-to-point, continuous  $\Rightarrow A$  closed

$\hookrightarrow A: X \rightarrow Y, \beta: Y \rightarrow Z$  point-set maps,  $C = \beta \circ A: X \rightarrow Z, C(x) = \bigcup_{y \in A(x)} \beta(y), A$  closed,  $\beta$  closed on  $A(x) = \bigcup_{x \in X} A(x)$ ,  $Y$  compact  $\Rightarrow C$  closed.

Global Convergence Theorem - Let  $A: X \rightarrow P(X)$  generate  $\{x_n\}$  arbitrarily by  $x_{n+1} \in A(x_n)$ , picking  $x_0 \in X$ . Let  $\Gamma \subseteq X$ :

$\{x_n\}$  compact ( $X$  compact or  $\{x_n\}$  bounded),  $Z: X \rightarrow \mathbb{R}$  descent function for  $A$  and  $\Gamma$ ,  $A$  closed  $\Rightarrow x_n \rightarrow x \in \Gamma$  (each subsequence of  $\{x_n\}$  converges to something in  $\Gamma$ )

Hilbert

## Line Search

Newton's Method -  $f \in C^2$ ,  $x^*$  min of  $f$ ,  $f'(x^*)=0$ ,  $f''(x^*) \neq 0$   $\Rightarrow$  close to  $x^* \Rightarrow \{x_k\}$  produced by Newton's method  $\rightarrow x^*$

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

False Position -  $g \in C^2$ ,  $g(x^*)=0$ ,  $g'(x^*) \neq 0$ ,  $x_0$  close to  $x^* \Rightarrow \{x_k\}$  produced by  $\text{FP} \rightarrow x^*$

$$x_{k+1} = x_k - g(x_k) \left[ \frac{x_k - x_{k-1}}{g(x_k) - g(x_{k-1})} \right]$$

Quadratic Fit -  $F \in C^2$ ,  $F$  unimodal. Find  $x_1 < x_2 < x_3$  w/  $f(x_1), f(x_2), f(x_3)$   $\Rightarrow x^* \in [x_1, x_3]$

General  $\mathcal{S}: E^n \rightarrow P(E)$   $\mathcal{S}(\vec{x}, \vec{d}) = \{\vec{y} | \vec{y} = \vec{x} + \vec{d}, d \geq 0 \text{ and } f(\vec{y}) = \min_{0 \leq d < \infty} f(\vec{x} + \vec{d})\}$

$\hookrightarrow f$  continuous  $\Rightarrow \mathcal{S}$  closed at points  $(\vec{x}, \vec{d}), \vec{d} \neq \vec{0}$ .

## Stopping Criteria

Percentage test - Stop when  $|x_k - x^{*}| \leq C\alpha^k$ ,  $f(\vec{x} + \vec{d}^*) = \min_{0 \leq d < \infty} \{f(\vec{x} + \vec{d})\} \rightarrow$  Need exact min to be on line, but don't need to know  $d^*$ !

Armijo, Goldstein, Wolfe - other tests which decide if estimate of  $d^*$  too high or low.

$A = \text{SoG}$ ,  $G(\vec{x}) = (\vec{x} - g(\vec{x}))$  ( $g$  = gradient),  $\Gamma = \{\vec{x} | \nabla f(\vec{x}) = 0\}$ ,  $Z(\vec{x}) = f(\vec{x})$   $\rightarrow$  descent function  
 $\{x_k\}$  bounded  $\Rightarrow A$  converges.

## Order of Convergence

$\{r_k\} \rightarrow r^*$  order  $\{r_k\}$  is largest  $p \geq 0$   $\lim_{k \rightarrow \infty} \frac{|r_{k+1} - r^*|}{|r_k - r^*|^p} < \infty$  linear convergence:  $p=1$ ,  $\lim_{k \rightarrow \infty} \frac{|r_{k+1} - r^*|}{|r_k - r^*|} = \beta < 1$  speed of convergence (smaller = better)

$\lim_{k \rightarrow \infty} \frac{r_{k+1}}{r_k^p} = C > 0 \Rightarrow$  order of convergence is  $p$  and  $r_{k+1} \approx Cr_k^p$  (large  $p$ , small  $C$  = faster convergence).

for Quadratic  $f(\vec{x}) = \frac{1}{2} \vec{x}^\top Q \vec{x} + \vec{b}^\top \vec{x}$ ,  $Q$  pos. def, symmetric.  $\exists!$  global min =  $Q^{-1}\vec{b}$  order of convergence 2 and  $\beta = \frac{(A-A)^2}{(A+A)^2}$   $A \rightarrow$  largest e-value  
 $\alpha = \frac{A}{\alpha} \otimes R.O.C$  unaffected by choice of  $x_0$ , only depends on  $\alpha, A$ .  $\alpha$  and  $A$   $\rightarrow$  smaller  $\alpha$ , larger  $A$ .  $= \frac{(1-\alpha)^2}{1+\alpha}$

Convex Combination -  $\alpha_1 y_1 + \dots + \alpha_n y_n$ ,  $\alpha_i \geq 0$ ,  $\sum \alpha_i = 1$ ,  $\in$  Convex hull of  $y_i$ 's.

Non-Quadratic Use Hessian of  $f(\vec{x})$ ,  $\{x_k\} \rightarrow x^* \leftarrow$  relative min, Order of convergence = 1, R.O.C. =  $\frac{(A-A)^2}{(A+A)^2}$   $A \rightarrow$  largest e-value of  $Q(\vec{x})$   $\alpha \rightarrow$  smallest e-value of  $Q(\vec{x})$

## Newton's Method

$x_{k+1} = x_k - (F(x_k))^{-1} \nabla F(x_k)^\top$  [Compare w/ 1st var  $x_{k+1} = x_k - f''(x_k)^{-1} f'(x_k)$ ]

$\rightarrow$  if  $f \in C^3$ ,  $x^*$  rel. min,  $F(x^*)$  pos-def,  $x_0$  close to  $x^* \Rightarrow \{x_k\} \rightarrow x^*$  w/ order of convergence 2.

$x_{k+1} = x_k - \alpha_k M_k \nabla F(x_k)^\top$  Steepest descent:  $\alpha_k$  output of  $\mathcal{S}$ ,  $M_k = I_n$

N.M:  $\alpha_k = 1$ ,  $M_k = F^{-1}(x_k)$   $\rightarrow$  vector determining direction of descent.

$\rightarrow$  for from  $x^* \rightarrow$  large  $\alpha_k \rightarrow$  act like grad descent.  
 $\rightarrow M_k \rightarrow$  pumps up diagonal  $\rightarrow$  near  $x^* \rightarrow$  small  $\alpha_k \rightarrow$  act like N.M.

## Levenberg-Maquardt

Modified NM,  $x_{k+1} = x_k - \alpha_k (\epsilon_k I + F(x_k))^{-1} \nabla F(x_k)^\top$  choose  $\epsilon_k > 0$  and get e-values of  $F(x_k)$ , pick  $\epsilon_k =$  smallest constant so  $\epsilon_k I + F(x_k)$  has all e-values  $> \epsilon$ . Need large  $\epsilon$  so that far from  $x^*$  looks like  $F(x_k)$  [N.M.], not too small or e-values close to 0 and numerically unstable.

Travel in direction  $\vec{e}_i, -\vec{e}_i$  (ith basis vector) at each step, How to chose direction?  $\rightarrow$  cyclic!  $1, 2, \dots, n, 1, 2, \dots \rightarrow$  Double sweep:  $1, 2, \dots, n, n-1, \dots, 2, 1$

$\rightarrow$  Rank 1  $\rightarrow$  Gauss-Southwell: pick  $\vec{e}_i$  steepest according to  $\nabla F(x_k)$ ,  $\{x_k\} \rightarrow x^*$  if  $f \in C^1$ ,  $n-1$  iterations = 1 iteration of steepest descent.

$\rightarrow$  fix algorithm C w/  $Z(C(x)) \leq Z(x)$ , Z descent function. C may not converge to solution, or too complex to analyze.

Apply another algorithm B which does converge, apply B instead of C every fixed # of steps infinitely often, then this will converge.

$\rightarrow x_k \rightarrow x_{k+1} : x_{k+1} \in B(x_k)$  instead of  $x_{k+1} \in C(x_k)$ .

## Space Steps

Neg def = local max  
pos def = local min

Gram-Schmidt Process: begin with  $v_1, \dots, v_K$  linearly indep vectors:

$$\text{Let } u_1 = v_1 \quad \text{and then } e_1 = \frac{v_1}{\|v_1\|}$$

$$u_k = v_k - \sum_{j=1}^{k-1} \text{Proj}_{u_j}(v_j) = v_k - \sum_{j=1}^{k-1} \frac{\langle v_k, u_j \rangle}{\|u_j\|^2} u_j$$

### Conjugate Direction Methods

$Q$  pos. def., Symmetric  $n \times n$  matrix  $u, v \in \mathbb{C}^n$ ,  $u, v$   $Q$ -orthogonal  $\Leftrightarrow u^T Q v = 0$ .  $\{d_1, \dots, d_n\}$   $Q$ -orthogonal  $\Leftrightarrow d_i^T Q d_j = 0 \forall i \neq j \leq n$

$Q$  orthogonal  $\Rightarrow$  linear indep.

- If  $f(x) = \frac{1}{2} x^T Q x - b^T x$ ,  $Qx^* = b$ , for  $\{d_1, \dots, d_n\}$   $Q$ -orthogonal,  $x^* = \sum_{i=1}^{n-1} d_i^T b / \|d_i\|^2$ ,  $d_i = \frac{b^T d_i}{d_i^T Q d_i}$

- taking  $x_{K+1} = x_K - d_K d_K^T$ ,  $d_K = \frac{g_K^T g_K}{g_K^T Q g_K}$ ,  $g_K = Qx_K - b$ ,  $\{x_K\} \rightarrow x^*$  ( $W L Qx^* = b$ ) in  $n$  steps.  $x^* = \sum_{K=0}^{n-1} \frac{d_K^T g_K}{d_K^T Q d_K} d_K$

Conjugate Gradient Method - Start at  $x_0$ , let  $d_0 = -g_0 = -(Qx_0 - b)$ ,  $x_{K+1} = x_K + d_K d_K^T$ ,  $d_K = -g_K^T(x_K) d_K / g_K^T Q d_K$

$\hookrightarrow x_n = x^*$ , each  $x_K$  minimizes  $f$  on  $x_0 + B_K = \text{span}\{d_0, \dots, d_{K-1}\}$ ,  $d_{K+1} = -g_{K+1} + \beta_K d_K$ ,  $g_K = Qx_K - b$ ,  $\beta_K = \frac{g_K^T Q d_K}{g_{K+1}^T Q d_K}$   
 $\forall K, \{d_0, \dots, d_K\}$  will be  $Q$ -conjugate.  $\beta_K = \frac{g_{K+1}^T g_{K+1}}{g_K^T g_K}$ , Converges in  $n$  steps for  $f$  quadratic!

Naive - let  $g_K = \nabla f(x_K) \rightarrow$  expensive, doesn't converge.

Nonquadratic Case - Partial CGM - Reset  $x_0$  to  $x_i$  every  $n$  steps:  $d_i = -g(x_i)$

Fletcher-Reeves -  $d_0 = -g_0$ ,  $x_{K+1} = x_K - d_K d_K^T$ ,  $d_{K+1} = -g_{K+1} + \beta_K d_K$ ,  $\beta_K = \frac{g_{K+1}^T g_{K+1}}{g_K^T g_K}$

Quasi-Newton Methods -  $x_{K+1} = x_K - d_K S_K \nabla F^T(x_K)$ ,  $S_K \approx F(x)^{-1}$  quadratic -  $S_K$  pos. def., symmetric,  $\text{Rate} = \lim_{K \rightarrow \infty} \frac{(B_K - B_K)^2}{B_K}$ ,  $B_K$  max/min eigenvalues of  $S_K Q$ .

Approximate  $F^{-1}$  Rank 1 correction -  $H_{K+1} = H_K + (P_K - H_K q_K)(P_K - H_K q_K)^T / q_K^T (P_K - H_K q_K)$ ,  $H_K \rightarrow F^{-1}$  in  $\leq n$  steps, since  $P_i = H_{K+i} q_i$ ,  $i \leq K$

$p_K = x_{K+1} - x_K$ ,  $q_K = g_{K+1} - g_K \Rightarrow q_K \approx F P_K^{-1}$  \* true def. only if  $q^T (P - H_K q_K) > 0$ , not guaranteed! Can have numerical issues.  
(rank 2 correction)

DFP - Start w/ symmetric pos. def. matrix  $H_0$ ,  $x_0$ , ①  $d_K = -H_K g_K$  ②  $\min_f(x + t d_K) = d_K$ , get  $x_{K+1}$ ,  $B_{K+1}$ , let,  $P_K = d_K d_K^T$

③ set  $q_K = g_{K+1} - g_K$ ,  $H_{K+1} = H_K + \frac{P_K P_K^T}{P_K^T q_K} - \frac{H_K q_K q_K^T H_K}{q_K^T H_K q_K}$  \* preserves the def.,  $P_K$  are  $F$ -conjugate  $\Rightarrow$  is a conjugate directions method.

Broyden - satisfy  $q_i = F^{-1} p_i$ : instead of  $F^{-1} q_i = p_i$ . Generate  $B_{K+1}$  from  $B_K$  using Complementary formula from  $H_K$  to  $H_K$ , swapping  $P_i$  with  $q_i$  and  $H_K$  with  $B_K$ .

pure: pick  $\epsilon \in \mathbb{R}$ ,  $H_{K+1}^P = (1-\epsilon) H_{K+1} + \epsilon P_K$  DFP  $\xrightarrow{\text{BFGS version of DFP}}$  and  $\epsilon = 0 \Rightarrow \text{DFP}$ ,  $\epsilon = 1 \Rightarrow \text{BFGS}$ .

non pure: Don't pick  $\epsilon$  in advance, have a sequence  $\{\epsilon_i\}$   $\neq d_K = \min_f(x_K + d_K d_K)$   $\Rightarrow$  All Broyden meth. produce exactly the same  $x_{K+1}$ !

Lagrange Multipliers -  $\min_f(\vec{x})$  subject to  $\vec{h}(\vec{x}) = (h_i(\vec{x}))_{i=1}^m = 0$ ,  $\vec{g}(\vec{x}) = (g_j(\vec{x}))_{j=1}^p \leq 0$ ,  $\vec{x} \in E^n$ ,  $m, n, f, g_j, h_i \in C^2$

Active Constraints - restrict feasible directions at  $x^*$ , since  $x^*$  at boundary of  $\{x | g_j(x) \leq 0\}$ , inactive  $\Rightarrow x \in \{x | g_j(x) < 0\}$  (interior point)

regular point = local max

regular point -  $x^*$  w/  $h(x^*) = 0 \wedge \nabla h_i(x^*) \cdots \nabla h_m(x^*) \perp I$ .

1st order nec. conditions  $\Rightarrow$  Solve n-m eqns  $h_i(x^*) = 0$  w.r.t  $\lambda, x^*$  Change to Jacobi form  $\begin{bmatrix} y_1 \\ \vdots \\ y_p \end{bmatrix} \nabla h(x^*) y = 0$   $\begin{bmatrix} 2nd \text{ order sufficient condition} \end{bmatrix}$

2nd order nec. conditions  $\Rightarrow x^*$  solves n-m eqns and  $\nabla^2 f(x^*) + \lambda^T \nabla^2 h(x^*)$  positive semi-definite on tangent plane of  $h$  at  $x^*$

↳ find orthonormal Basis  $E$  of  $M$ ,  $L_M \in E$ , check if  $L_M$  pos. def.

OR ↳ solve  $P(\lambda) = \det \begin{bmatrix} 0 & \nabla h \\ -\nabla^T h & L - \lambda I \end{bmatrix}_{n \times n}$ . Each  $\lambda$  is an eigenvalue of  $L_M$ .

OR ↳ Bordered Hessian Test  $\Rightarrow L_M$  pos. def.  $\Leftrightarrow$  last  $n-m$  principal minors of  $\begin{bmatrix} 0 & \nabla h \\ \nabla^T h & L \end{bmatrix}_{n \times n}$  have sign  $(-1)^m$

### KKT Conditions

If  $\vec{x}^*$  is a point of constraint set  $K$ , which is a local min of  $f$  on  $K \Rightarrow \exists \lambda \in E^m, \exists \mu \in E^p$ ,  $\nabla f(\vec{x}^*) + \lambda^T \nabla h(\vec{x}^*) + \mu^T \nabla g(\vec{x}^*) = 0$ , with  $\vec{\lambda} \geq 0$  s.t.  
and  $\mu^T g(\vec{x}^*) = 0$ .

Hilroy

Modified Newton's Method - Globally Convergent in finitely Many Steps [Quadratic Case]

(order > 1) (order 1)  
finite > Superlinear > linear

Lem. - R.O.C =  $\lim_{K \rightarrow \infty} \frac{(b_K - b_K)^2}{b_K + b_K}$  B<sub>K</sub>, b<sub>K</sub> largest, smallest evals of M<sub>K</sub> ∇<sup>2</sup>f(x\*) [Nonquadratic Case]

→ must be the definite to guarantee this as a descent method for small α.

General formula:  $x_{k+1} = x_k - \alpha_k M_k^{-1} \nabla f(x_k)$

**Steepest Descent** A = I<sub>n</sub> ∇<sup>2</sup>f

→ d<sub>k</sub> output of S, M<sub>K</sub> = I<sub>n</sub>

→ Convergence → Globally Convergent

→ Order 1, R.O.C =  $\left(\frac{A-\alpha}{A+\alpha}\right)^2$  [Non Quadratic]  
A, α largest + smallest evals of ∇<sup>2</sup>f(x\*)

→  $f(x_{k+1}) - f(x^*) \leq \left(1 - \frac{\alpha}{A}\right)(f(x_k) - f^*)$

↳ S.D. makes progress even when far from soln!  
↳ inexact the search doesn't change the rate much!

**Coordinate Descent**

→ ignore d<sub>k</sub> M<sub>K</sub> ∇<sup>2</sup>f(x<sub>k</sub>)<sup>T</sup>, use e<sub>i</sub> (or -e<sub>i</sub>)  
→ Global convergence

→ Convergence - slower than S.D. (1 step S.D. = n-1 steps C.D.)

→ Easy to implement.

**Partial Conjugate Gradient**

→ faster than S.D. less inflexible than N.M.

→ Idea: Can get d<sub>k</sub> from Q-conj dir w/o x\*, using b, (Qx\* = b)

→ more efficient as movement along d<sub>k</sub> will not undo progress made in previous iterations → each step makes more progress than

→ d<sub>k</sub> : Step of S.D.

→ conjugate gradient procedure carried out for m+n steps,

→ then restarting from current point for m+n more steps taken.

→ n steps [Quadratic]

**Quadratic Approximation** Set starting matrix as I<sub>n</sub>

→ g<sub>k</sub> ≈ ∇f(x<sub>k</sub>)<sup>T</sup>, Q ≈ ∇<sup>2</sup>f(x<sub>k</sub>)

→ after n-1 steps restart and do pure gradient step, every n steps

→ No line search

→ F(x<sub>k</sub>) evaluated at each point, impractical! not globally

Convergent! [Non quadratic]

**Line Search Methods** Use line search in place of computing ∇<sup>2</sup>f(x<sub>k</sub>)

→ Globally Convergent, or each restart 3 or 4 steps of gradient descent (3/4 step super)

→ Converge linear, R.O.C. dependent on E vals of ∇<sup>2</sup>f(x\*) [Non-quadratic]

**Broyden-Fletcher-Goldfarb-Shanno (BFGS)**

→ Complementary formula for DFP, then invert becomes resulting  $\nabla^2 f(x)$  to DFP  $\nabla^2 f(x)$ !

→ Superior performance to DFP.

**Pure** - uses fixed ϕ.

- Convergence - superlinear when viewed in blocks of m steps, which approx 1-step MP conj. dir. → Convergence may be slow if m large.

- sensitive to line search inaccuracies.

**Impure** - uses sequence of {ϕ<sub>k</sub>}

R.O.C =  $\lim_{K \rightarrow \infty} \frac{(b_K - b_K)^2}{b_K + b_K}$  B<sub>K</sub>, b<sub>K</sub> largest, smallest evals of M<sub>K</sub> ∇<sup>2</sup>f(x\*) [Nonquadratic Case]

→ must be the definite to guarantee this as a descent method for small α.

**Newton's Method**

→ d<sub>k</sub> = 1, M<sub>K</sub> = [∇<sup>2</sup>f(x<sub>k</sub>)<sup>-1</sup>]

→ Convergence - locally Convergent

- Order 2 (faster than S.D.)

→ Need to ensure M<sub>K</sub> positive definite, or

→ d<sub>k</sub> M<sub>K</sub> ∇<sup>2</sup>f(x<sub>k</sub>)<sup>T</sup> may change sign and move away from min! Storage of ∇<sup>2</sup>f(x<sub>k</sub>)<sup>-1</sup> costly!

→ Sensitive to E-value\* Structure of Hessian, trouble if Hessian hard to compute.

**Levenberg-Maquardt**

→ Let M<sub>K</sub> = [E<sub>K</sub>I<sub>n</sub> + ∇<sup>2</sup>f(x<sub>k</sub>)<sup>-1</sup>]

↳ Small ε → M<sub>K</sub> ≈ ∇<sup>2</sup>f(x<sub>k</sub>)<sup>-1</sup> ↳ fast convergence near soln since like N.M. Near x\*

↳ Large ε → M<sub>K</sub> ≈ E<sub>K</sub> ∇<sup>2</sup>f(x<sub>k</sub>)<sup>-1</sup> ↳ global convergence since like S.D. far from x\* Ctr Def!

Convergence - Global, order 2 near x\*, Contingent on ε.

**Quasi-Newton Methods**

→ use gradient and that  $g(x_{k+1}) - g(x_k) \nabla^2 f(x_k)^{-1} = (x_{k+1} - x_k)$   
→ And  $\nabla^2 f(x_n) \approx Q$  Equality if P Qinv →  $\nabla^2 f(x^*) = Q$   
Then use Newton's method w/ this approx.

Convergence - global if restarted every n steps, as each restart begins w/ a S.D. step (sparses step)

↳ superlinear as approximated C.B.M, but takes n steps to get from x<sub>k</sub> to x<sub>k+1</sub>. (Slow for large n)

↳ sensitive to E-values, inaccurate line searches.

**Rank One Correction**

→ update  $\nabla^2 f(x_j)$  w/ rank 1 matrix maintaining symmetry and

→ May not preserve the def of  $\nabla^2 f(x_j)$

→ uses  $\nabla^2 f(x_j)$  in line search to get d<sub>j</sub>.

→ Numerical issues w/ small #s.

**Rank Two Correction - DFP**

→ update  $\nabla^2 f(x_j)$  w/ rank 2 matrix maintaining symmetry, the def and

→  $\{(g_{k+1} - g_k) \nabla^2 f(x_k)^{-1}\}$  produced are  $\nabla^2 f$  conjugate dir method!

Convergence - n steps [Quadratic]

**Broyden Family** - All produce same x<sub>n+1</sub> if  $d_{k+1} = \min_{\alpha} (f_k + \alpha d_k)$

→ satisfy  $(g(x_{k+1}) - g(x_k)) = \nabla^2 f(x_k)(x_{k+1} - x_k)$  instead of

→ update Broyden with complementary formula (swap g(x<sub>j</sub>) w/ x<sub>j</sub>), or take inverse of  $\nabla^2 f(x_k)^{-1}$ .

→ Both BFGS and DFP have symmetric rank 2 corrections, so  $\nabla^2 f(x)$  is symmetric and satisfies

$\nabla^2 f(x) = (1-\phi) \nabla^2 f(x) + \phi \nabla^2 f(x)$  DFP BFGS

↳ preserves symmetry, if  $\phi \geq 0$  also preserves the def.

General Line Search Algorithm  $S: E^n \rightarrow P(E^n)$ ,  $S(\vec{x}, \vec{d}) = \{\vec{y} \mid \vec{y} = \vec{x} + \alpha \vec{d}, \alpha \geq 0, f(\vec{y}) = \min_{0 \leq \alpha \leq \infty} f(\vec{x} + \alpha \vec{d})\}$

$\rightarrow$  minimize over a line in direction of vector  $\vec{d}$ . Assume unimodal.

Curve fitting  $\rightarrow$  minimize over polynomial approximation of curve.

$\rightarrow$  locally convergent even w/ 3-pt pattern

$\rightarrow$  Newton Method  $\rightarrow x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$

$\rightarrow f \in C^2, f''(x_k) \neq 0, f'(x_k) = 0$  or else won't converge.  $f''(x_k) > 0$ .

Method of false position  $\rightarrow$  replace  $f''(x_k)$  with  $\frac{f(x_{k+1}) - f(x_k)}{x_{k+1} - x_k}$ .

$\rightarrow$  Same convergence as N.M.

$\rightarrow f \in C^1$

Cubic fit  $\rightarrow$  minimize over cubic approximation of curve.

$\rightarrow$  faster convergence than above but needs  $f'(x_k), (f \in C^1)$ .

Quadratic fit  $\rightarrow$  minimize over quadratic approximation of curve.

$\rightarrow$  does not use  $f''(x_k)$ , only  $x_{k-2}, x_{k-1}, x_k$

$\rightarrow$  can be globally convergent if use 3-pt pattern:  $(x_1, x_2, x_3)$  where

$x_1 < x_2 < x_3 \wedge f(x_1), f(x_3) \geq f(x_2)$

Use QF and maintain pattern to ensure convergence.

Stopping criteria  $\rightarrow$  percentage test, Armijo test, etc...

$\rightarrow$  determine what is too high and too low for estimate of  $\alpha$ .