3.4 Newton's method

Near a strict local minimizer $\bar{x}$ we approximate $f \in C^2$ by the quadratic

$$q(x) = f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2} (x - x_k)^T \underbrace{H(x_k)}_{\nabla^2 f(x_k)} (x - x_k)$$

$$\nabla q(x) = \nabla f(x_k) + H(x_k)(x - x_k)$$

Since $H(\bar{x})$ pos. def., $H(x_k)$ is pos. def. if x_k is close to $\bar{x}$ by continuity. Hence, $H(x_k)^{-1}$ exists (and is pos. def.!).

Define the next point x_{k+1} by

$$\nabla q(x_{k+1}) = 0 \iff \nabla f(x_k) + H(x_k)(x_{k+1} - x_k) = 0$$

$$\iff x_{k+1} = x_k \underbrace{- H(x_k)^{-1} \nabla f(x_k)}_{d_k}$$

no line search ($\lambda_k = 1$)

Def. d is a descent direction at x if

(*) $f(x + \lambda d) < f(x)$ for small $\lambda > 0$

$$\Rightarrow \frac{f(x + \lambda d) - f(x)}{\lambda} < 0 \quad \text{— " —}$$

let $\lambda \to 0 \Rightarrow f'(x; d) = \underline{\nabla f(x)^T d \leq 0}$

necessary condition

(*) $f(x+\lambda d) < f(x)$ $\forall$ small $\lambda > 0$

$\Leftrightarrow$ $f(x) + \lambda \nabla f(x)^T d + o(\lambda) < f(x)$ -"-

$\Leftrightarrow$ $\lambda \left(\underbrace{\nabla f(x)^T d}_{\text{fixed}} + \underbrace{o(1)}_{\to 0} \right) < 0$ -"-

sufficient condition $\nabla f(x)^T d < 0$

Newton: $d_k = -H(x_k)^{-1} \nabla f(x_k)$ gives

$$\nabla f(x_k)^T d = -\nabla f(x)^T \underbrace{H(x_k)^{-1}}_{\text{pos. def.}} \nabla f(x_k) < 0$$

Thus d_k is a descent direction if

$H(x_k)$ is pos. def.

Lemma: H pos. def. with eigenvalues

$0 < \lambda_{min} \leq \dots \leq \lambda_{max} \Rightarrow \lambda_{min} \|x\| \leq \|Hx\| \leq \lambda_{max} \|x\|$.

Proof: λ is eigenvalue of $H \Rightarrow \lambda^2$ eigenv. of H^2

Use spectral thm: $x = Q\hat{x}$, $Q^T H^2 Q = \Lambda^2$

$$\|Hx\|^2 = (Hx)^T Hx = x^T H^2 x = (Q\hat{x})^T H^2 (Q\hat{x}) = \hat{x}^T Q^T H^2 Q \hat{x}$$

$$= \hat{x}^T \Lambda^2 \hat{x} = \sum \lambda_i^2 \hat{x}_i^2 \begin{cases} \geq \lambda_{min}^2 \|\hat{x}\|^2 = \lambda_{min}^2 \|x\|^2 \\ \leq \lambda_{max}^2 \|x\|^2 \end{cases} \quad \#$$

Thm 2: If $f \in C^3$, $\nabla f(\bar{x}) = 0$, $H(\bar{x})$ pos. def.

then there exists ($\exists$) a neighbourhood $\Omega \ni \bar{x}$:

$$x_1 \in \Omega \Rightarrow \|x_{k+1} - \bar{x}\| < C \|x_k - \bar{x}\|^2 \quad \forall k$$

(C: constant)

i.e. $x_k \to \bar{x}$ as $k \to \infty$ with

second-order convergence.

Proof: $x_{k+1} = x_k - H(x_k)^{-1} \nabla f(x_k)$ $\Leftrightarrow$

$$\underbrace{x_{k+1} - \bar{x}}_{\delta_{k+1}} = \underbrace{x_k - \bar{x}}_{\delta_k} - H_k^{-1} g_k$$

(a) $\delta_{k+1} = \delta_k - H_k^{-1} g_k$

Taylor expansion of the gradient at x_k (Exerc. 1.7)

$$\nabla f(x) = \nabla f(x_k) + H_k (x - x_k) + \mathcal{O}(\|x - x_k\|^2)$$

$$x = \bar{x} \Rightarrow \quad 0 = g_k - H_k \delta_k + \mathcal{O}(\|\delta_k\|^2)$$

(a) $\Leftrightarrow$ $H_k \delta_{k+1} = H_k \delta_k - g_k$

$$H_k \delta_{k+1} = \underbrace{H_k \delta_k - H_k \delta_k}_{=0} + \mathcal{O}(\|\delta_k\|^2)$$

$\Rightarrow$ $\|H_k \delta_{k+1}\| = \mathcal{O}(\|\delta_k\|^2) \leq K \|\delta_k\|^2$ for $x_k \in \Omega_1 \ni \bar{x}$

Lemma gives $\lambda_{min}(x_k) \|\delta_{k+1}\| \leq \|H_k \delta_{k+1}\| \leq K \|\delta_k\|^2$ —"—

Choose $\Omega_2 \ni \bar{x}$: $0 < L \leq \lambda_{min}(x_k)$

then $\|\delta_{k+1}\| \leq \frac{K}{L} \|\delta_k\|^2 = \underbrace{\frac{K}{L} \|\delta_k\|}_{< M < 1 \text{ in } \Omega_3 \ni \bar{x}} \|\delta_k\|$

Let $\Omega = \Omega_1 \cap \Omega_2 \cap \Omega_3$

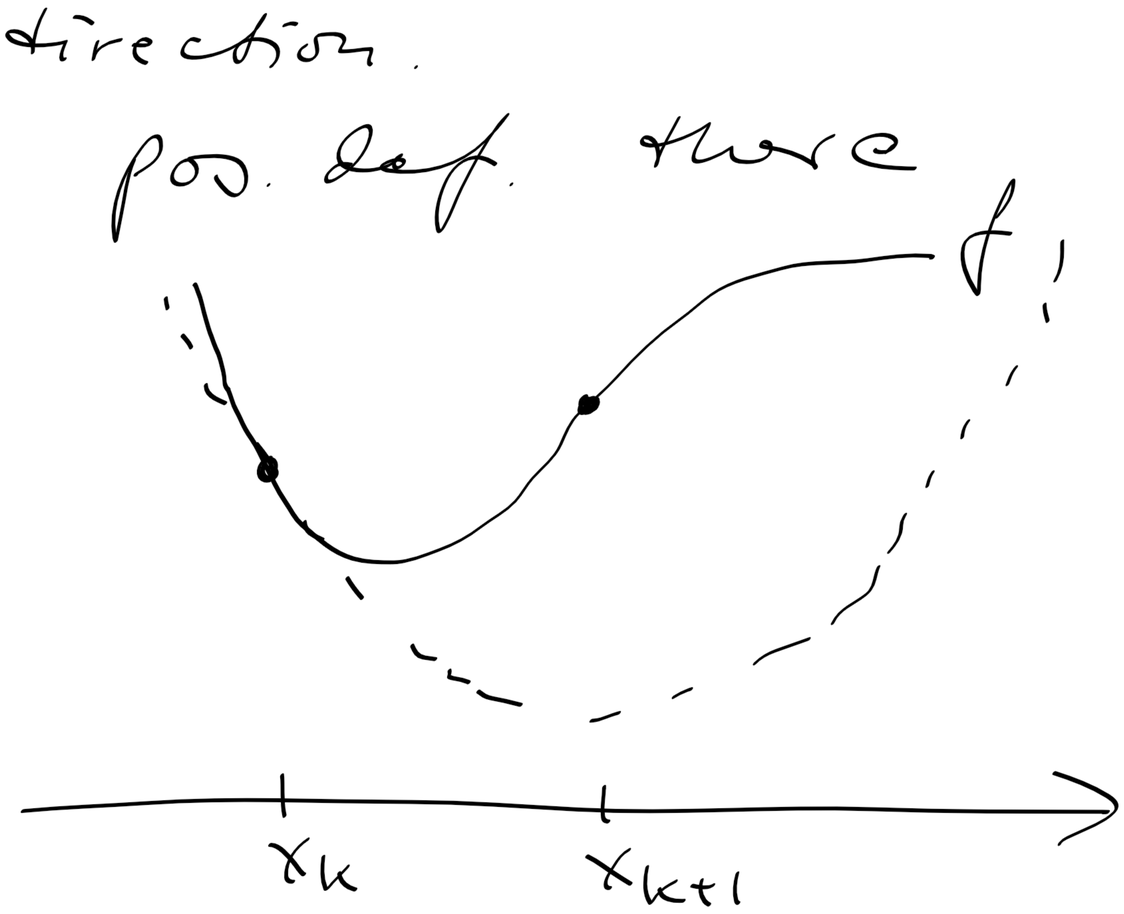
$$\|x_{k+1} - \bar{x}\| < M \|x_k - \bar{x}\| < M^k \|x_1 - \bar{x}\| \to 0, \; k \to \infty$$

#

⊕ Fast convergence

⊖ • Must start close to a minizer, otherwise $d_k = -H_k^{-1} g_k$ may not be a descent direction.

• Even if H_k is pos. def. there may be problem:



• Second-order derivatives needed

Modified Newton methods

- Use line search in the direction

$$d_k = -H(x_k)^{-1} \nabla f(x_k)$$

- If $H(x_k)$ is not pos. def., then solve

$$\left(H(x_k) + \varepsilon_k I\right) d_k = -\nabla f(x_k)$$

for $\varepsilon_k > 0$ that makes $H(x_k) + \varepsilon_k I$ pos. def.

Note: ε_k large $\Rightarrow$ almost steepest descent

In implementations you don't compute inverses, but factorize, e.g. Cholesky:

$$H(x_k) + \varepsilon_k I = L L^T, \qquad L = \left(\boxed{\times}\ 0\right)$$

$$L \underbrace{L^T d}_{z} = -\nabla f \iff \begin{cases} Lz = -\nabla f \\ L^T d = z \end{cases}$$

- Use $d_k = -B_k \nabla f(x_k)$

with B_k is pos. def. updated on every iteration. No second derivative needed. Quasi-Newton methods

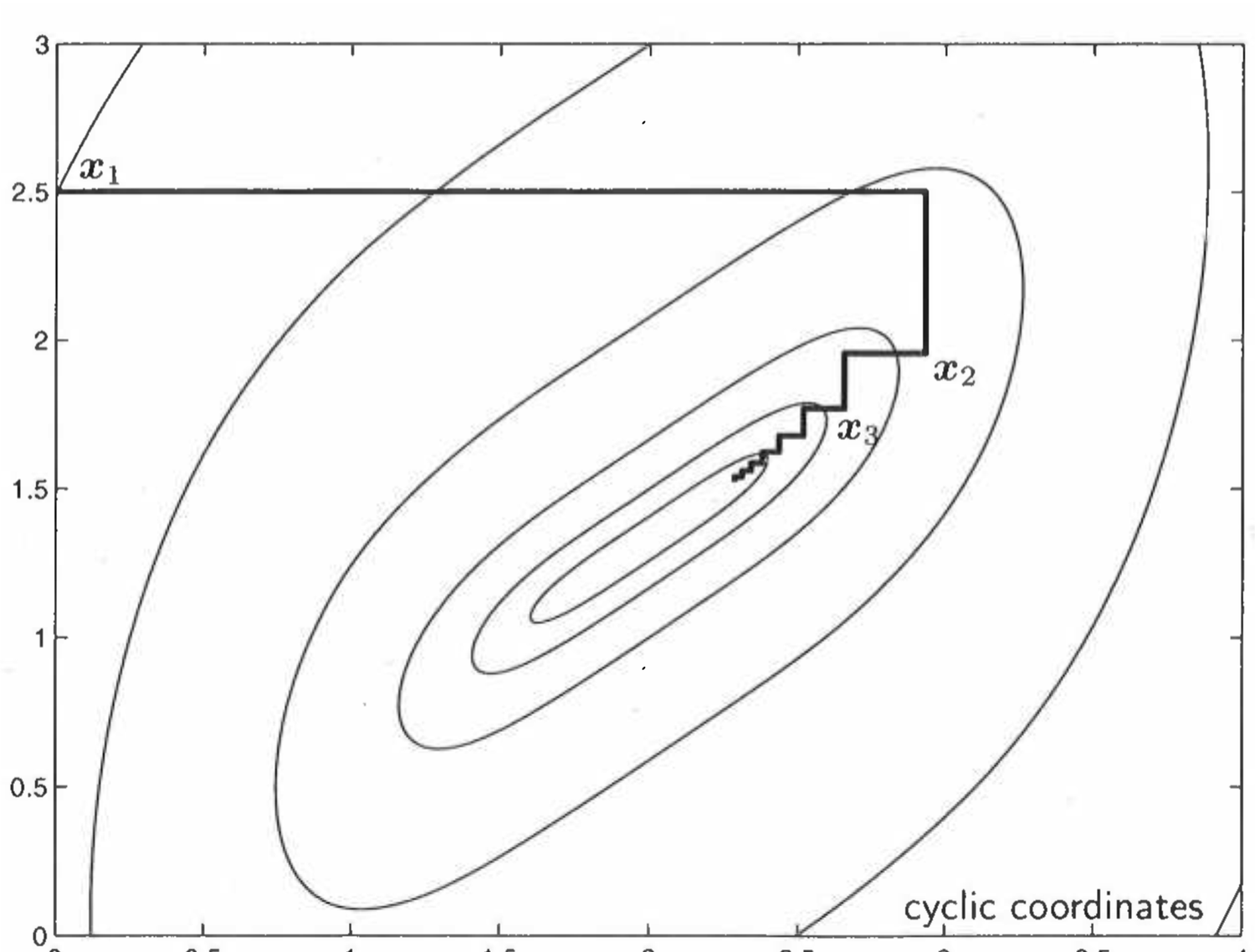
3.2 Cyclic-coordinates search

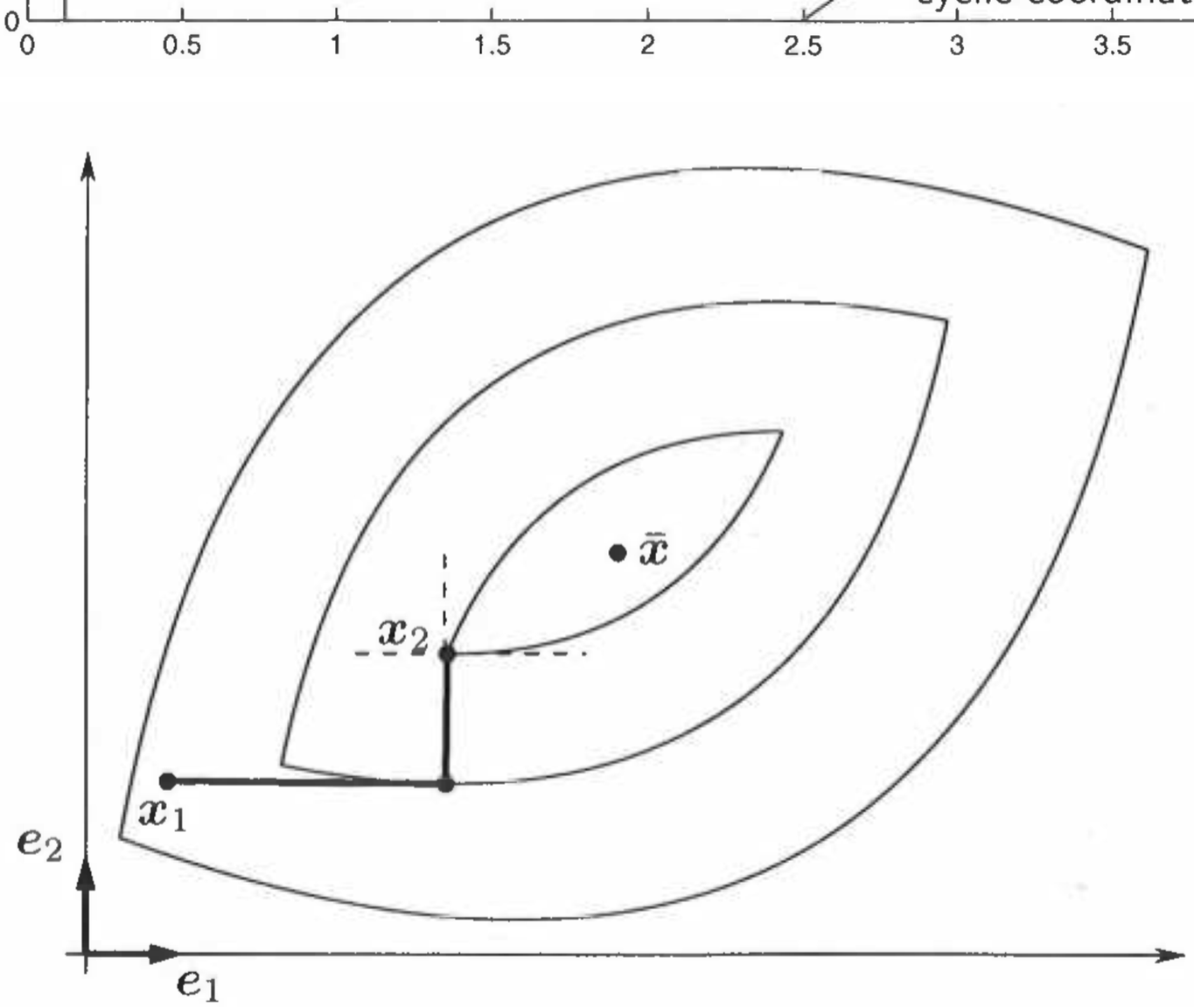
Use canonical base $e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, e_2, \ldots, e_n, e_1, \ldots$

as search directions plus line search.

⊕ Simple, no derivatives needed, can be used on non-differentiable functions.

⊖ Slow, can get stuck.





3.7 Nelder-Mead simplex method

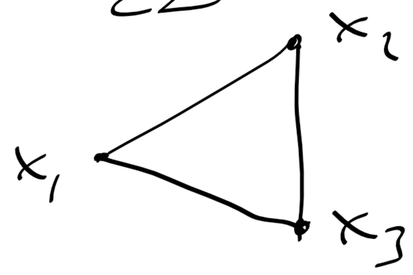
A simplex in $\mathbb{R}^n$ is a set of $n+1$ points $x_1, \dots, x_{n+1}$ such that the vectors

$x_i - x_1$, $i = 2, \dots, n+1$, are linearly independent.

1D

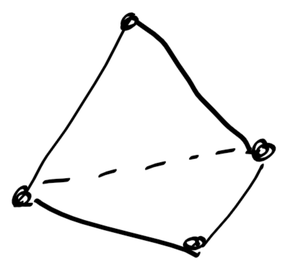
interval

2D



triangle

3D



tetrahedron

Compares function values $f(x_i)$

⊕ Robust, no derivatives needed

⊖ Slow