Newton step

$$\Delta x_{\rm nt} = -\nabla^2 f(x)^{-1} \nabla f(x)$$

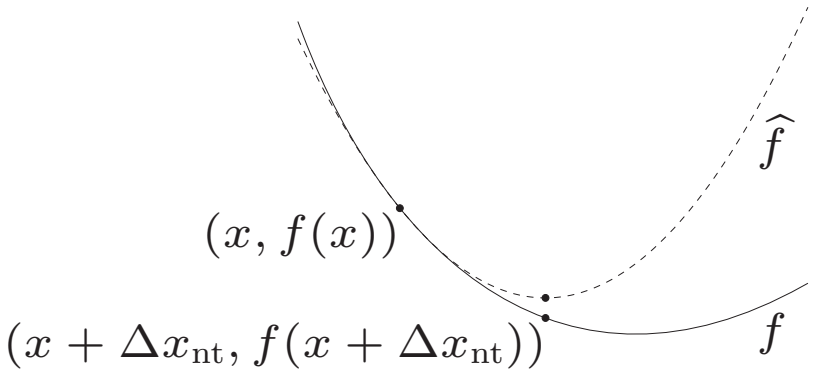
interpretations If $f(x)$ is a quadratic, $x + \Delta x_{\rm nt}$ is the minimizer

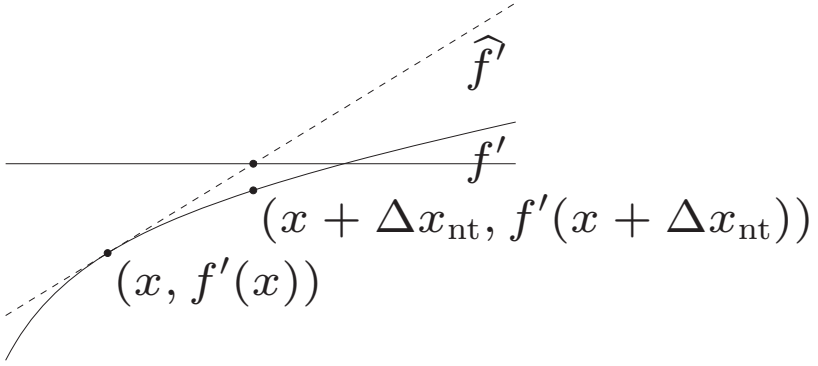
- $x + \Delta x_{\rm nt}$ minimizes second order approximation

$$\widehat{f}(x+v) = f(x) + \nabla f(x)^T v + \frac{1}{2} v^T \nabla^2 f(x) v$$

- $x + \Delta x_{\rm nt}$ solves linearized optimality condition

$$\nabla f(x+v) \approx \nabla \widehat{f}(x+v) = \nabla f(x) + \nabla^2 f(x) v = 0$$

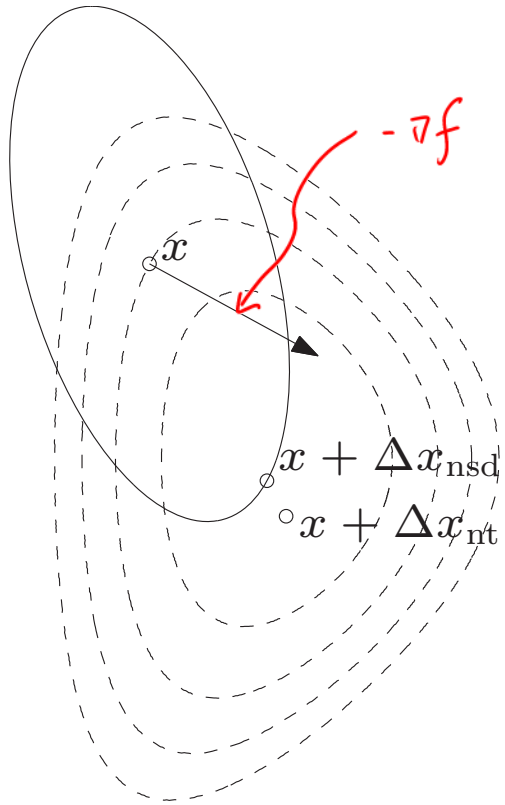




$\nabla f^T \Delta x_{nt} = -\nabla f^T \nabla^2 f^{-1} \nabla f < 0$ unless $\nabla f = 0$ assuming f is convex.

- $\Delta x_{\rm nt}$ is steepest descent direction at x in local Hessian norm Δx_{nt} may not be descent for nonconvex f

$$\|u\|_{\nabla^2 f(x)} = \left(u^T \nabla^2 f(x) u\right)^{1/2}$$



dashed lines are contour lines of f; ellipse is $\{x + v \mid v^T \nabla^2 f(x) v = 1\}$

arrow shows $-\nabla f(x)$

Newton decrement

$$\lambda(x) = \left(\nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x)\right)^{1/2}$$

a measure of the proximity of x to $x^\star$

properties

- gives an estimate of $f(x) - p^\star$, using quadratic approximation $\widehat{f}$:

$$f(x) - \inf_y \widehat{f}(y) = \frac{1}{2}\lambda(x)^2$$

- equal to the norm of the Newton step in the quadratic Hessian norm

$$\lambda(x) = \left(\Delta x_{\rm nt}^T \nabla^2 f(x) \Delta x_{\rm nt}\right)^{1/2}$$

- directional derivative in the Newton direction: $\nabla f(x)^T \Delta x_{\rm nt} = -\lambda(x)^2$
- affine invariant (unlike $\|\nabla f(x)\|_2$)

Newton step: independent of linear change of coordinates

Assume $T \in \mathbb{R}^{n \times n}$ is nonsingular.

Let $\bar{f} = f(Ty)$. $x = Ty$. Then

$$\nabla \bar{f} = T^T \nabla f \qquad \nabla^2 \bar{f} = T^T \nabla^2 f \, T$$

$$\Delta y_{nt} = -(T^T \nabla^2 f \, T)^{-1} \cdot T^T \nabla f$$

$$= -T^{-1} \nabla^2 f \, \nabla f$$

$$= T^{-1} \Delta x_{nt}$$

$$\Rightarrow \quad x + \Delta x_{nt} = T(y + \Delta y_{nt})$$

i.e. Newton steps of f and $\bar{f}$ are related by the same linear transformation

- This property does not hold for gradient descent

Newton's method

---

given a starting point $x \in \mathbf{dom}\, f$, tolerance $\epsilon > 0$.
repeat

1. *Compute the Newton step and decrement.*
   $\Delta x_{\rm nt} := -\nabla^2 f(x)^{-1}\nabla f(x)$; $\quad \lambda^2 := \nabla f(x)^T \nabla^2 f(x)^{-1}\nabla f(x)$.
2. *Stopping criterion.* **quit** if $\lambda^2/2 \leq \epsilon$.
3. *Line search.* Choose step size t by backtracking line search.
4. *Update.* $x := x + t\Delta x_{\rm nt}$.

---

affine invariant, *i.e.*, independent of linear changes of coordinates:

Newton iterates for $\tilde{f}(y) = f(Ty)$ with starting point $y^{(0)} = T^{-1}x^{(0)}$ are

$$y^{(k)} = T^{-1}x^{(k)}$$

Classical convergence analysis

assumptions

- f strongly convex on S with constant m
- $\nabla^2 f$ is Lipschitz continuous on S, with constant $L > 0$:

$$\|\nabla^2 f(x) - \nabla^2 f(y)\|_2 \leq L\|x - y\|_2$$

bound on the third derivative

(L measures how well f can be approximated by a quadratic function)

e.g., $L = 0$ if $f(x)$ is a quadratic

outline: there exist constants $\eta \in (0, m^2/L)$, $\gamma > 0$ such that

- if $\|\nabla f(x)\|_2 \geq \eta$, then $f(x^{(k+1)}) - f(x^{(k)}) \leq -\gamma$
- if $\|\nabla f(x)\|_2 < \eta$, then

$$\frac{L}{2m^2}\|\nabla f(x^{(k+1)})\|_2 \leq \left(\frac{L}{2m^2}\|\nabla f(x^{(k)})\|_2\right)^2$$

← quadratic convergence region

damped Newton phase ($\|\nabla f(x)\|_2 \geq \eta$)

- most iterations require backtracking steps
- function value decreases by at least γ
- if $p^\star > -\infty$, this phase ends after at most $(f(x^{(0)}) - p^\star)/\gamma$ iterations

quadratically convergent phase ($\|\nabla f(x)\|_2 < \eta$)

- all iterations use step size $t = 1$
- $\|\nabla f(x)\|_2$ converges to zero quadratically: if $\|\nabla f(x^{(k)})\|_2 < \eta$, then

$$\frac{L}{2m^2}\|\nabla f(x^l)\|_2 \leq \left(\frac{L}{2m^2}\|\nabla f(x^k)\|_2\right)^{2^{l-k}} \leq \left(\frac{1}{2}\right)^{2^{l-k}}, \qquad l \geq k$$

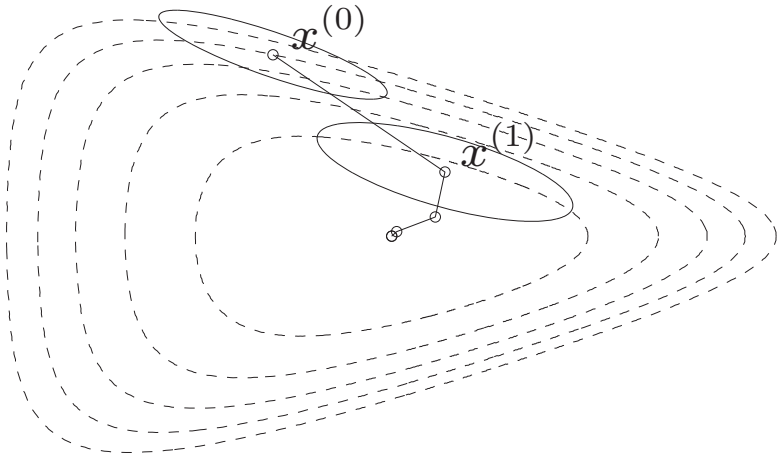
conclusion: number of iterations until $f(x) - p^\star \leq \epsilon$ is bounded above by

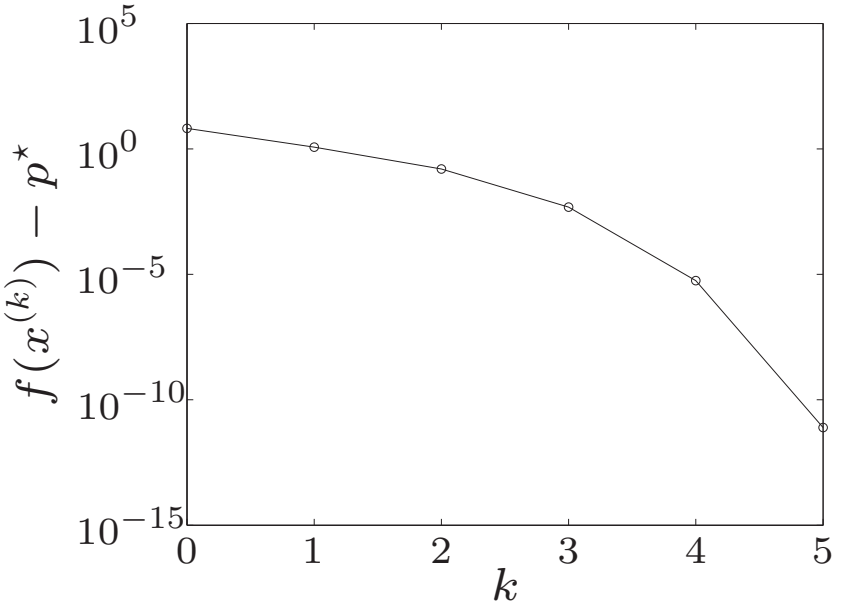
$$\frac{f(x^{(0)}) - p^\star}{\gamma} + \log_2 \log_2(\epsilon_0/\epsilon)$$

- γ, ϵ_0 are constants that depend on m, L, $x^{(0)}$
- second term is small (of the order of 6) and almost constant for practical purposes
- in practice, constants m, L (hence γ, ϵ_0) are usually unknown
- provides qualitative insight in convergence properties ($i.e.$, explains two algorithm phases)

Examples

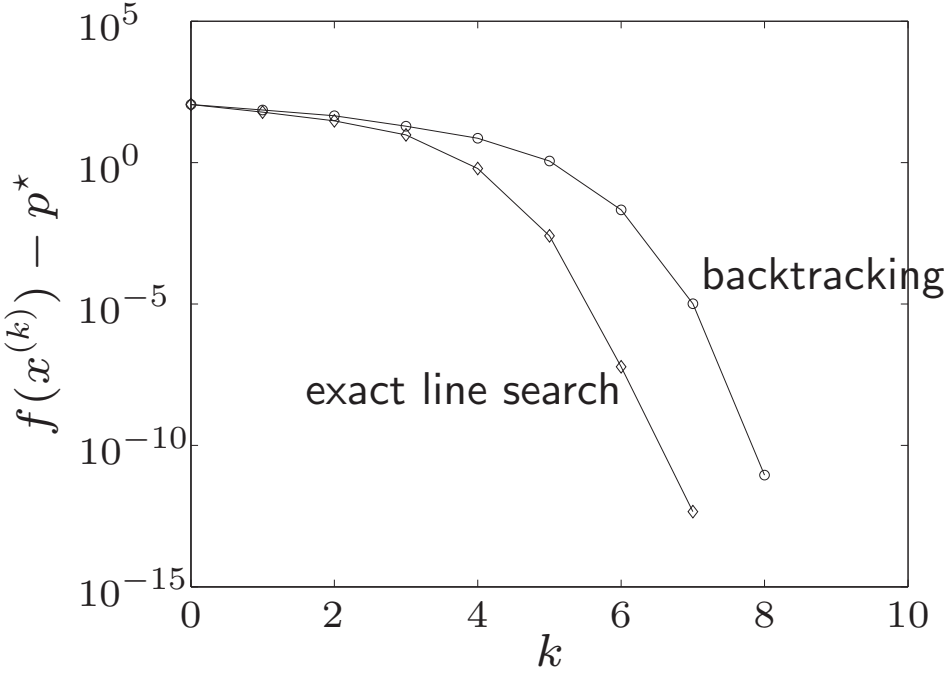
example in $\mathbf{R}^2$ (page 10–9)

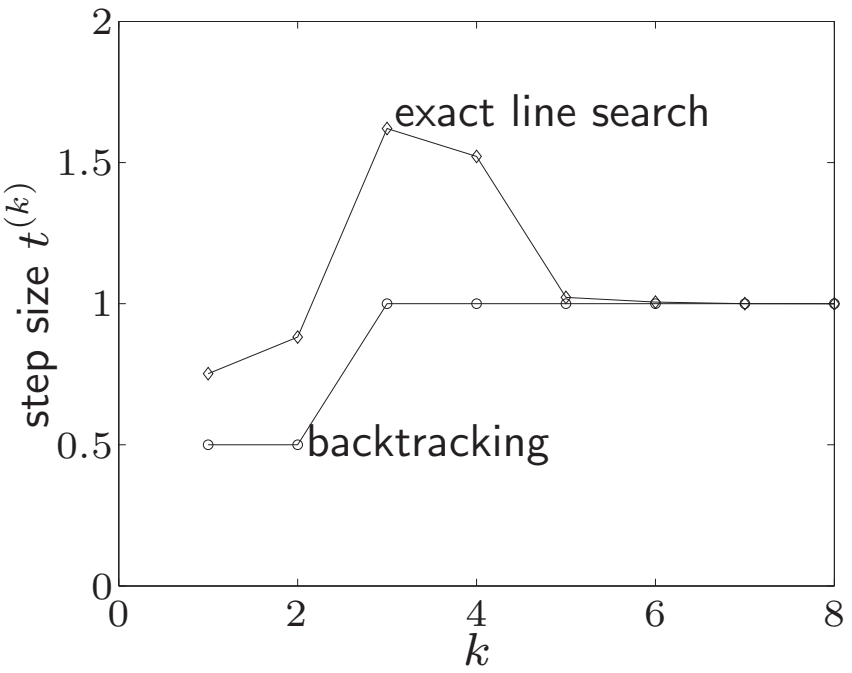




- backtracking parameters $\alpha = 0.1$, $\beta = 0.7$
- converges in only 5 steps
- quadratic local convergence

example in $\mathbf{R}^{100}$ (page 10–10)

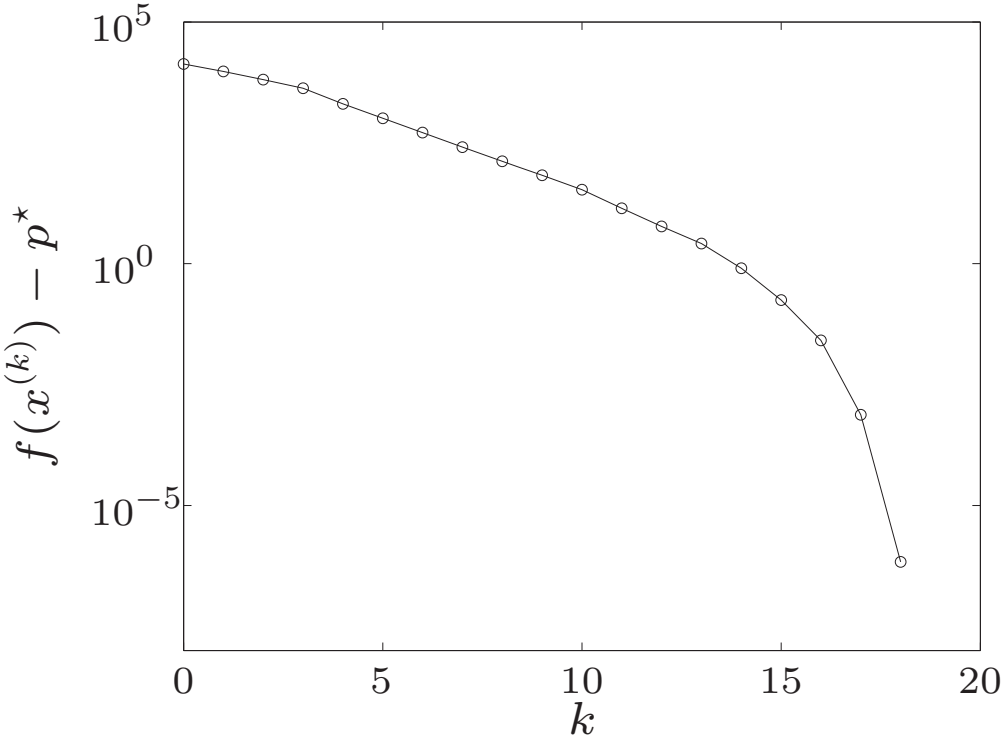




- backtracking parameters $\alpha = 0.01$, $\beta = 0.5$
- backtracking line search almost as fast as exact l.s. (and much simpler)
- clearly shows two phases in algorithm

example in $\mathbf{R}^{10000}$ (with sparse a_i)

$$f(x) = -\sum_{i=1}^{10000} \log(1 - x_i^2) - \sum_{i=1}^{100000} \log(b_i - a_i^T x)$$



- backtracking parameters $\alpha = 0.01$, $\beta = 0.5$.
- performance similar as for small examples

Summary of Newton's Method

- Convergence is typically fast once the algorithm enters the quadratic convergence phase; which depends on $\eta \leq m^2/L$. If η is very small, quadratic convergence regim can be small
- Affine invariant
- scales well with prob. size

Disadvantage:

- computation requires
  - evaluation of $\nabla^2 f$
  - solve $\nabla^2 f \, d = -\nabla f$

Self-concordance

shortcomings of classical convergence analysis

- depends on unknown constants (m, L, . . .)
- bound is not affinely invariant, although Newton's method is

convergence analysis via self-concordance (Nesterov and Nemirovski)

- does not depend on any unknown constants
- gives affine-invariant bound
- applies to special class of convex functions ('self-concordant' functions)
- developed to analyze polynomial-time interior-point methods for convex optimization

Self-concordant functions

chosen for convenience
If $|f'''(x)| \le K f''(x)^{3/2}$
$\tilde{f}(x) = K^2/4 f(x)$ is s.c. follow definition

definition

- convex $f : \mathbf{R} \to \mathbf{R}$ is self-concordant if $|f'''(x)| \le 2f''(x)^{3/2}$ for all $x \in \mathbf{dom}\, f$
- $f : \mathbf{R}^n \to \mathbf{R}$ is self-concordant if $g(t) = f(x + tv)$ is self-concordant for all $x \in \mathbf{dom}\, f$, $v \in \mathbf{R}^n$

$f: \mathbf{R}^n \to \mathbf{R}$ is self-concordant if it is s.c. along every line

examples on R

- linear and quadratic functions
- negative logarithm $f(x) = -\log x$
- negative entropy plus negative logarithm: $f(x) = x \log x - \log x$

affine invariance: if $f : \mathbf{R} \to \mathbf{R}$ is s.c., then $\tilde{f}(y) = f(ay + b)$ is s.c.:

$$\tilde{f}'''(y) = a^3 f'''(ay + b), \qquad \tilde{f}''(y) = a^2 f''(ay + b)$$

Self-concordant calculus

properties

- preserved under positive scaling $\alpha \geq 1$, and sum
- preserved under composition with affine function
- if g is convex with $\mathbf{dom}\, g = \mathbf{R}_{++}$ and $|g'''(x)| \leq 3g''(x)/x$ then

$$f(x) = \log(-g(x)) - \log x$$

  is self-concordant

examples: properties can be used to show that the following are s.c.

- $f(x) = -\sum_{i=1}^{m} \log(b_i - a_i^T x)$ on $\{x \mid a_i^T x < b_i,\ i = 1, \ldots, m\}$
- $f(X) = -\log\det X$ on $\mathbf{S}_{++}^n$
- $f(x) = -\log(y^2 - x^T x)$ on $\{(x, y) \mid \|x\|_2 < y\}$

Convergence analysis for self-concordant functions

summary: there exist constants $\eta \in (0, 1/4]$, $\gamma > 0$ such that

- if $\lambda(x) > \eta$, then
$$f(x^{(k+1)}) - f(x^{(k)}) \leq -\gamma$$
- if $\lambda(x) \leq \eta$, then
$$2\lambda(x^{(k+1)}) \leq \left(2\lambda(x^{(k)})\right)^2$$

(η and γ only depend on backtracking parameters α, β)

complexity bound: number of Newton iterations bounded by

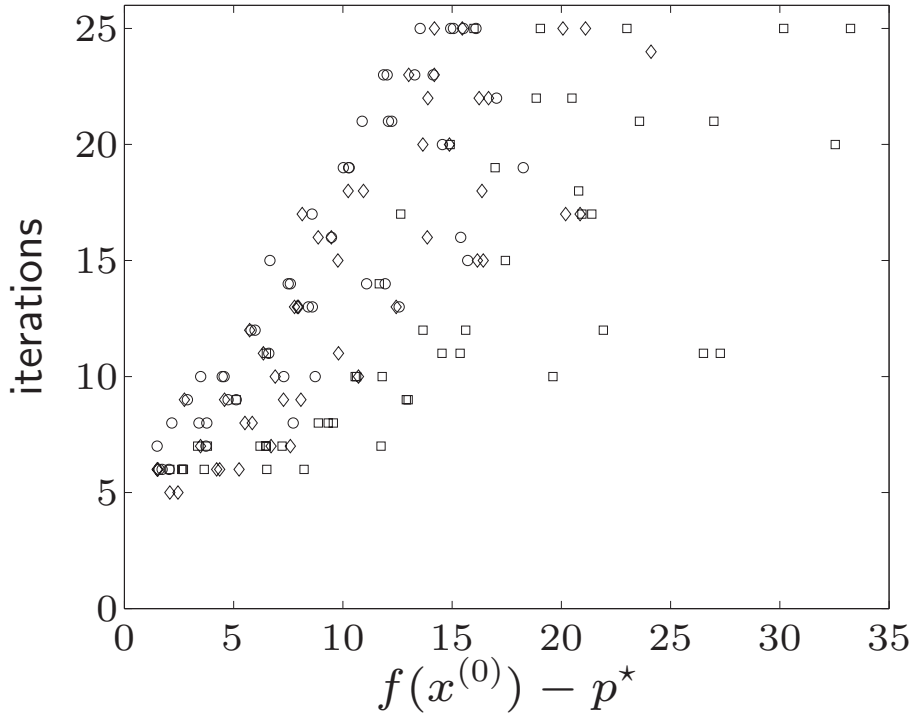
$$\frac{f(x^{(0)}) - p^\star}{\gamma} + \log_2 \log_2(1/\epsilon)$$

for $\alpha = 0.1$, $\beta = 0.8$, $\epsilon = 10^{-10}$, bound evaluates to $375(f(x^{(0)}) - p^\star) + 6$

numerical example: 150 randomly generated instances of

$$\text{minimize} \quad f(x) = -\sum_{i=1}^m \log(b_i - a_i^T x)$$

$\bigcirc$: $m = 100$, $n = 50$
$\square$: $m = 1000$, $n = 500$
$\Diamond$: $m = 1000$, $n = 50$



- number of iterations much smaller than $375(f(x^{(0)}) - p^\star) + 6$
- bound of the form $c(f(x^{(0)}) - p^\star) + 6$ with smaller c (empirically) valid

Implementation

main effort in each iteration: evaluate derivatives and solve Newton system

$$H\Delta x = g$$

where $H = \nabla^2 f(x)$, $g = -\nabla f(x)$

via Cholesky factorization

$$H = LL^T, \qquad \Delta x_{\rm nt} = L^{-T}L^{-1}g, \qquad \lambda(x) = \|L^{-1}g\|_2$$

- cost $(1/3)n^3$ flops for unstructured system
- cost $\ll (1/3)n^3$ if H sparse, banded

example of dense Newton system with structure

$$f(x) = \sum_{i=1}^{n} \psi_i(x_i) + \psi_0(Ax + b), \qquad H = D + A^T H_0 A$$

- assume $A \in \mathbf{R}^{p \times n}$, dense, with $p \ll n$
- D diagonal with diagonal elements $\psi_i''(x_i)$; $H_0 = \nabla^2 \psi_0(Ax + b)$

method 1: form H, solve via dense Cholesky factorization: (cost $(1/3)n^3$)

method 2 (page 9–15): factor $H_0 = L_0 L_0^T$; write Newton system as

$$D\Delta x + A^T L_0 w = -g, \qquad L_0^T A \Delta x - w = 0$$

eliminate Δx from first equation; compute w and Δx from

$$(I + L_0^T A D^{-1} A^T L_0) w = -L_0^T A D^{-1} g, \qquad D\Delta x = -g - A^T L_0 w$$

cost: $2p^2 n$ (dominated by computation of $L_0^T A D^{-1} A^T L_0$)