Convex Optimization

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9. Unconstrained minimization

Outline

Terminology and assumptions

Gradient descent method

Steepest descent method

Newton's method

Self-concordant functions

Implementation

Unconstrained minimization

- unconstrained minimization problem

$$\text{minimize} \quad f(x)$$

- we assume
  - f convex, twice continuously differentiable (hence $\mathbf{dom}\, f$ open)
  - optimal value $p^\star = \inf_x f(x)$ is attained at $x^\star$ (not necessarily unique)
- optimality condition is $\nabla f(x) = 0$
- minimizing f is the same as solving $\nabla f(x) = 0$
- a set of n equations with n unknowns

Quadratic functions

- convex quadratic: $f(x) = (1/2)x^T Px + q^T x + r$, $P \succeq 0$
- we can solve exactly via linear equations

$$\nabla f(x) = Px + q = 0$$

- much more on this special case later

Iterative methods

- for most non-quadratic functions, we use **iterative methods**
- these produce a sequence of points $x^{(k)} \in \mathbf{dom}\, f$, $k = 0, 1, \ldots$
- $x^{(0)}$ is the **initial point** or **starting point**
- $x^{(k)}$ is the kth **iterate**
- we hope that the method **converges**, *i.e.*,

$$f(x^{(k)}) \to p^\star, \qquad \nabla f(x^{(k)}) \to 0$$

Initial point and sublevel set

- algorithms in this chapter require a starting point $x^{(0)}$ such that
  - $x^{(0)} \in \mathbf{dom}\, f$
  - sublevel set $S = \{x \mid f(x) \leq f(x^{(0)})\}$ is closed
- 2nd condition is hard to verify, except when **all** sublevel sets are closed
  - equivalent to condition that $\mathbf{epi}\, f$ is closed
  - true if $\mathbf{dom}\, f = \mathbf{R}^n$
  - true if $f(x) \to \infty$ as $x \to \mathbf{bd}\, \mathbf{dom}\, f$
- examples of differentiable functions with closed sublevel sets:

$$f(x) = \log\left(\sum_{i=1}^{m} \exp(a_i^T x + b_i)\right), \qquad f(x) = -\sum_{i=1}^{m} \log(b_i - a_i^T x)$$

Strong convexity and implications

- f is **strongly convex** on S if there exists an $m > 0$ such that

$$\nabla^2 f(x) \succeq mI \text{ for all } x \in S$$

- same as $f(x) - (m/2)\|x\|_2^2$ is convex
- if f is strongly convex, for $x, y \in S$,

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{m}{2}\|x - y\|_2^2$$

- hence, S is bounded
- we conclude $p^\star > -\infty$, and for $x \in S$,

$$f(x) - p^\star \leq \frac{1}{2m}\|\nabla f(x)\|_2^2$$

- useful as stopping criterion (if you know m, which usually you do not)

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Descent methods

- **descent methods** generate iterates as

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$

  with $f(x^{(k+1)}) < f(x^{(k)})$ (hence the name)

- other notations: $x^+ = x + t\Delta x$, $x := x + t\Delta x$
- $\Delta x^{(k)}$ is the **step**, or **search direction**
- $t^{(k)} > 0$ is the **step size**, or **step length**
- from convexity, $f(x^+) < f(x)$ implies $\nabla f(x)^T \Delta x < 0$
- this means Δx is a **descent direction**

Generic descent method

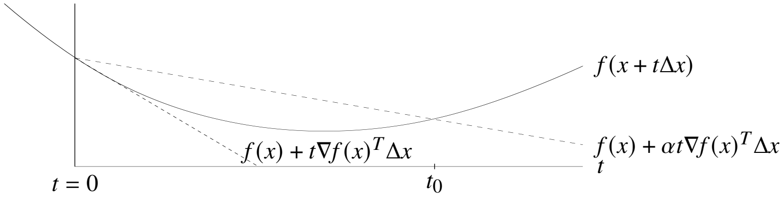
General descent method.

given a starting point $x \in \mathbf{dom}\, f$.
repeat
1. Determine a descent direction Δx.
2. **Line search.** Choose a step size $t > 0$.
3. **Update.** $x := x + t\Delta x$.

until stopping criterion is satisfied.

Line search types

- **exact line search:** $t = \text{argmin}_{t>0} f(x + t\Delta x)$
- **backtracking line search** (with parameters $\alpha \in (0, 1/2)$, $\beta \in (0, 1)$)
  - starting at $t = 1$, repeat $t := \beta t$ until $f(x + t\Delta x) < f(x) + \alpha t \nabla f(x)^T \Delta x$
- graphical interpretation: reduce t (*i.e.*, backtrack) until $t \leq t_0$



Gradient descent method

- general descent method with $\Delta x = -\nabla f(x)$

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given a starting point $x \in \textbf{dom}\, f$.
repeat
  1. $\Delta x := -\nabla f(x)$.
  2. **Line search.** Choose step size t via exact or backtracking line search.
  3. **Update.** $x := x + t\Delta x$.

until stopping criterion is satisfied.

- stopping criterion usually of the form $\|\nabla f(x)\|_2 \leq \epsilon$
- convergence result: for strongly convex f,

$$f(x^{(k)}) - p^\star \leq c^k (f(x^{(0)}) - p^\star)$$

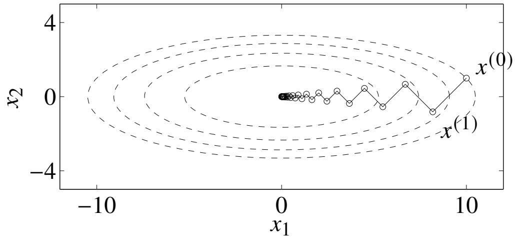
  $c \in (0, 1)$ depends on m, $x^{(0)}$, line search type
- very simple, but can be very slow

Example: Quadratic function on $\mathbf{R}^2$

- take $f(x) = (1/2)(x_1^2 + \gamma x_2^2)$, with $\gamma > 0$
- with exact line search, starting at $x^{(0)} = (\gamma, 1)$:

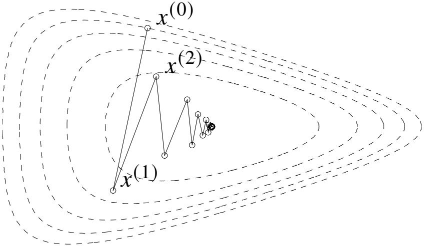
$$x_1^{(k)} = \gamma \left(\frac{\gamma - 1}{\gamma + 1}\right)^k, \qquad x_2^{(k)} = \left(-\frac{\gamma - 1}{\gamma + 1}\right)^k$$

  - very slow if $\gamma \gg 1$ or $\gamma \ll 1$
  - example for $\gamma = 10$ at right
  - called **zig-zagging**

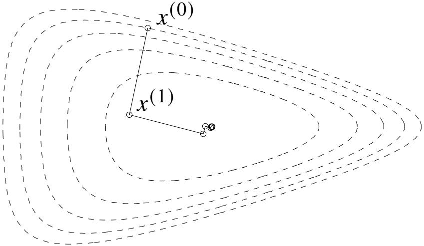


Example: Nonquadratic function on $\mathbf{R}^2$

- $f(x_1, x_2) = e^{x_1+3x_2-0.1} + e^{x_1-3x_2-0.1} + e^{-x_1-0.1}$



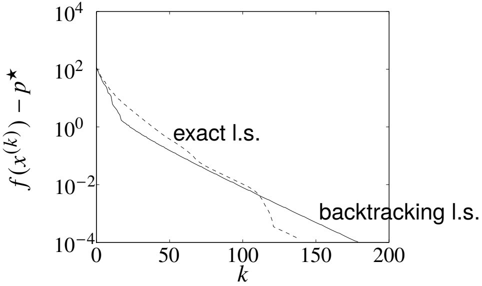
backtracking line search



exact line search

Example: A problem in $\mathbf{R}^{100}$

- $f(x) = c^T x - \sum_{i=1}^{500} \log(b_i - a_i^T x)$



- **linear convergence**, *i.e.*, a straight line on a semilog plot

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Steepest descent method

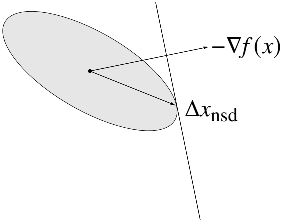
- **normalized steepest descent direction** (at x, for norm $\|\cdot\|$):

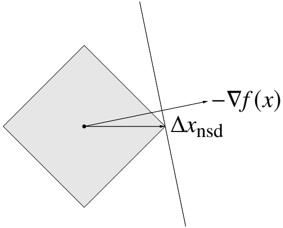
$$\Delta x_{\text{nsd}} = \operatorname{argmin}\{\nabla f(x)^T v \mid \|v\| = 1\}$$

- interpretation: for small v, $f(x+v) \approx f(x) + \nabla f(x)^T v$;
- direction Δx_{nsd} is unit-norm step with most negative directional derivative
- **(unnormalized) steepest descent direction**: $\Delta x_{\text{sd}} = \|\nabla f(x)\|_* \Delta x_{\text{nsd}}$
- satisfies $\nabla f(x)^T \Delta x_{\text{sd}} = -\|\nabla f(x)\|_*^2$
- **steepest descent method**
  - general descent method with $\Delta x = \Delta x_{\text{sd}}$
  - convergence properties similar to gradient descent

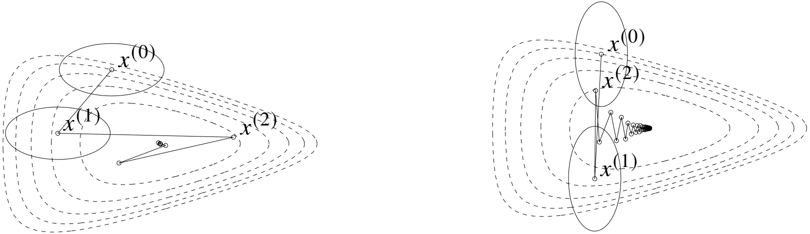
Examples

- Euclidean norm: $\Delta x_{\rm sd} = -\nabla f(x)$
- quadratic norm $\|x\|_P = (x^TPx)^{1/2}$ ($P \in \mathbf{S}^n_{++}$): $\Delta x_{\rm sd} = -P^{-1}\nabla f(x)$
- ℓ_1-norm: $\Delta x_{\rm sd} = -(\partial f(x)/\partial x_i)e_i$, where $|\partial f(x)/\partial x_i| = \|\nabla f(x)\|_\infty$
- unit balls, normalized steepest descent directions for quadratic norm and ℓ_1-norm:





Choice of norm for steepest descent



- steepest descent with backtracking line search for two quadratic norms
- ellipses show $\{x \mid \|x - x^{(k)}\|_P = 1\}$
- interpretation of steepest descent with quadratic norm $\|\cdot\|_P$: gradient descent after change of variables $\bar{x} = P^{1/2}x$
- shows choice of P has strong effect on speed of convergence

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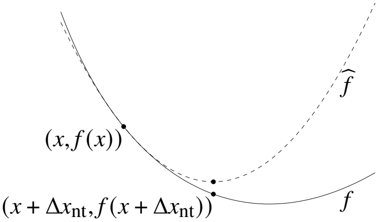
Newton step

- **Newton step** is $\Delta x_{\text{nt}} = -\nabla^2 f(x)^{-1} \nabla f(x)$
- **interpretation**: $x + \Delta x_{\text{nt}}$ minimizes second order approximation

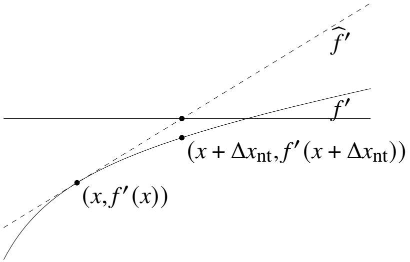
$$\widehat{f}(x+v) = f(x) + \nabla f(x)^T v + \frac{1}{2} v^T \nabla^2 f(x) v$$



Another intrepretation

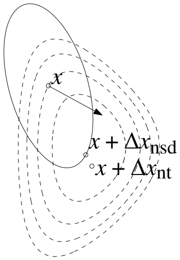
- $x + \Delta x_{\mathrm{nt}}$ solves linearized optimality condition

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



And one more interpretation

- Δx_{nt} is steepest descent direction at x in local Hessian norm $\|u\|_{\nabla^2 f(x)} = \left(u^T \nabla^2 f(x) u\right)^{1/2}$



- 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

- **Newton decrement** is $\lambda(x) = \left(\nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x)\right)^{1/2}$
- a measure of the proximity of x to $x^\star$
- 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

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

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

Newton's method

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

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

- **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 $L > 0$:

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

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

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

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

Classical convergence analysis

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

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

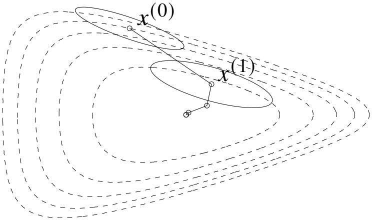
conclusion: number of iterations until $f(x) - p^\star \le \epsilon$ is bounded above by

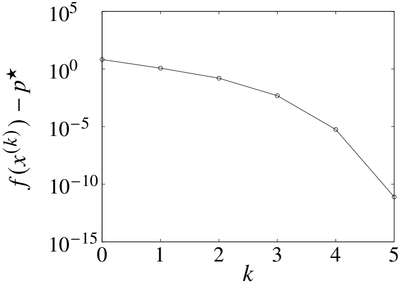
$$\frac{f(x^{(0)}) - p^\star}{\gamma} + \log_2 \log_2(\epsilon_0/\epsilon)$$

- 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)

Example: $\mathbf{R}^2$

(same problem as slide 9.13)

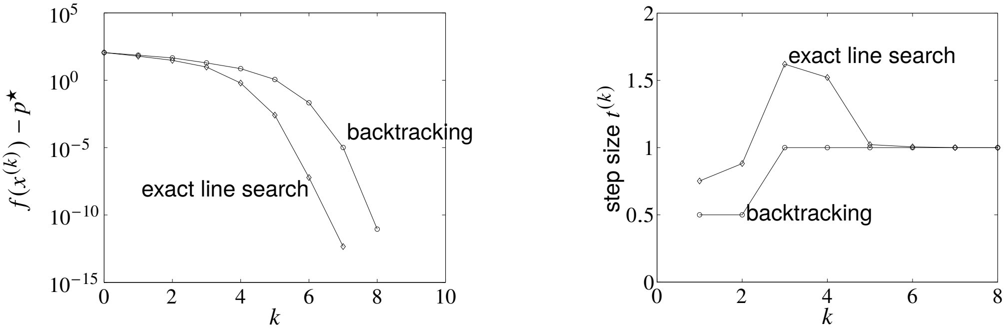




- backtracking parameters $\alpha = 0.1$, $\beta = 0.7$
- converges in only 5 steps
- quadratic local convergence

Example in $\mathbf{R}^{100}$

(same problem as page 9.14)

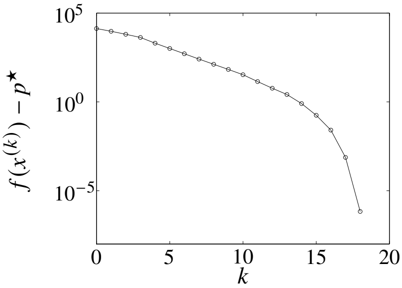


- backtracking parameters $\alpha = 0.01$, $\beta = 0.5$
- backtracking line search almost as fast as exact l.s. (and much simpler)
- clearly shows two phases in algorithm

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

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Self-concordance

shortcomings of classical convergence analysis

- depends on unknown constants $(m, L, \ldots)$
- 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

definition

- convex $f : \mathbf{R} \to \mathbf{R}$ is self-concordant if $|f'''(x)| \leq 2f''(x)^{3/2}$ 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 $x \in \mathbf{dom}\, f$, $v \in \mathbf{R}^n$

examples on $\mathbf{R}$

- 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

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

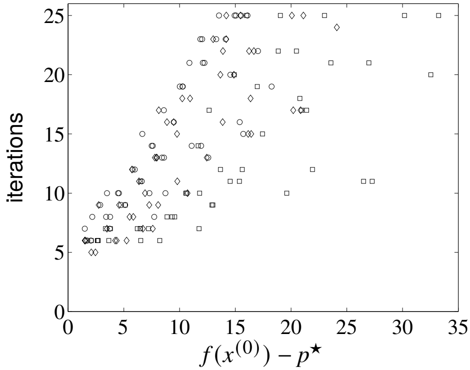
for $\alpha = 0.1$, $\beta = 0.8$, $\epsilon = 10^{-10}$, bound evaluates to $375(f(x^{(0)}) - p^\star) + 6$

Numerical example

150 randomly generated instances of

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

○: $m = 100$, $n = 50$
□: $m = 1000$, $n = 500$
◇: $m = 1000$, $n = 50$



- 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

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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

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

- 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 **??**): 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 $L_0^T A D^{-1} A^T L_0$)