Part 3: Trust-region methods for unconstrained optimization

Nick Gould (RAL)

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x)$$

Part C course on continuoue optimization

UNCONSTRAINED MINIMIZATION

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x)$$

where the **objective function** $f : \mathbb{R}^n \longrightarrow \mathbb{R}$

- ⊙ assume that $f \in C^1$ (sometimes C^2) and Lipschitz
- ⊙ often in practice this assumption violated, but not necessary

LINESEARCH VS TRUST-REGION METHODS

- **Linesearch methods**
  - pick descent direction p_k
  - pick stepsize α_k to "reduce" $f(x_k + \alpha p_k)$
  - $x_{k+1} = x_k + \alpha_k p_k$
- **Trust-region methods**
  - pick step s_k to reduce "model" of $f(x_k + s)$
  - accept $x_{k+1} = x_k + s_k$ if decrease in model inherited by $f(x_k + s_k)$
  - otherwise set $x_{k+1} = x_k$, "refine" model

TRUST-REGION MODEL PROBLEM

Model $f(x_k + s)$ by:

- linear model
$$m_k^L(s) = f_k + s^T g_k$$
- quadratic model — symmetric B_k
$$m_k^Q(s) = f_k + s^T g_k + \tfrac{1}{2} s^T B_k s$$

Major difficulties:

- models may not resemble $f(x_k + s)$ if s is large
- models may be unbounded from below
  - linear model - always unless $g_k = 0$
  - quadratic model - always if B_k is indefinite, possibly if B_k is only positive semi-definite

THE TRUST REGION

Prevent model $m_k(s)$ from unboundedness by imposing a **trust-region** constraint

$$\|s\| \leq \Delta_k$$

for some "suitable" scalar **radius** $\Delta_k > 0$

$\Longrightarrow$ **trust-region subproblem**

$$\text{approx} \quad \underset{s \in \mathbb{R}^n}{\text{minimize}} \; m_k(s) \; \text{ subject to } \; \|s\| \leq \Delta_k$$

- $\odot$ in theory does not depend on norm $\|\cdot\|$
- $\odot$ in practice it might!

OUR MODEL

For simplicity, concentrate on the second-order (Newton-like) model

$$m_k(s) = m_k^Q(s) = f_k + s^T g_k + \tfrac{1}{2} s^T B_k s$$

and the ℓ_2-trust region norm $\|\cdot\| = \|\cdot\|_2$

Note:

- $\odot$ $B_k = H_k$ is allowed
- $\odot$ analysis for other trust-region norms simply adds extra constants in following results

BASIC TRUST-REGION METHOD

Given $k = 0$, $\Delta_0 > 0$ and x_0, until "convergence" do:

Build the second-order model $m(s)$ of $f(x_k + s)$.

"Solve" the trust-region subproblem to find s_k for which $m(s_k)$ "<" f_k and $\|s_k\| \leq \Delta_k$, and define

$$\rho_k = \frac{f_k - f(x_k + s_k)}{f_k - m_k(s_k)}.$$

If $\rho_k \geq \eta_v$ [**very successful**] $\quad \boxed{0 < \eta_v < 1}$

set $x_{k+1} = x_k + s_k$ and $\Delta_{k+1} = \gamma_i \Delta_k$ $\quad \boxed{\gamma_i \geq 1}$

Otherwise if $\rho_k \geq \eta_s$ then [**successful**] $\quad \boxed{0 < \eta_s \leq \eta_v < 1}$

set $x_{k+1} = x_k + s_k$ and $\Delta_{k+1} = \Delta_k$

Otherwise [**unsuccessful**]

set $x_{k+1} = x_k$ and $\Delta_{k+1} = \gamma_d \Delta_k$ $\quad \boxed{0 < \gamma_d < 1}$

Increase k by 1

"SOLVE" THE TRUST REGION SUBPROBLEM?

At the very least

- aim to achieve as much reduction in the model as would an iteration of steepest descent
- **Cauchy point**: $s_k^{\mathrm{C}} = -\alpha_k^{\mathrm{C}} g_k$ where

$$\begin{aligned} \alpha_k^{\mathrm{C}} &= \underset{\alpha > 0}{\arg\min}\; m_k(-\alpha g_k) \;\text{ subject to }\; \alpha\|g_k\| \leq \Delta_k \\ &= \underset{0 < \alpha \leq \Delta_k/\|g_k\|}{\arg\min}\; m_k(-\alpha g_k) \end{aligned}$$

  - minimize quadratic on line segment $\Longrightarrow$ very easy!
- require that

$$m_k(s_k) \leq m_k(s_k^{\mathrm{C}}) \;\text{ and }\; \|s_k\| \leq \Delta_k$$

- in practice, hope to do far better than this

ACHIEVABLE MODEL DECREASE

Theorem 3.1. If $m_k(s)$ is the second-order model and $s_k^{\rm C}$ is its Cauchy point within the trust-region $\|s\| \leq \Delta_k$,

$$f_k - m_k(s_k^{\rm C}) \geq \tfrac{1}{2}\|g_k\| \min\left[\frac{\|g_k\|}{1+\|B_k\|}, \Delta_k\right].$$

PROOF OF THEOREM 3.1

$$m_k(-\alpha g_k) = f_k - \alpha\|g_k\|^2 + \tfrac{1}{2}\alpha^2 g_k^T B_k g_k.$$

Result immediate if $g_k = 0$.
Otherwise, 3 possibilities

(i) curvature $g_k^T B_k g_k \leq 0 \Longrightarrow m_k(-\alpha g_k)$ unbounded from below as α increases $\Longrightarrow$ Cauchy point occurs on the trust-region boundary.

(ii) curvature $g_k^T B_k g_k > 0$ & minimizer $m_k(-\alpha g_k)$ occurs at or beyond the trust-region boundary $\Longrightarrow$ Cauchy point occurs on the trust-region boundary.

(iii) the curvature $g_k^T B_k g_k > 0$ & minimizer $m_k(-\alpha g_k)$, and hence Cauchy point, occurs before trust-region is reached.

Consider each case in turn;

Case (i)

$g_k^T B_k g_k \le 0$ & $\alpha \ge 0 \Longrightarrow$

$$m_k(-\alpha g_k) = f_k - \alpha\|g_k\|^2 + \tfrac{1}{2}\alpha^2 g_k^T B_k g_k \le f_k - \alpha\|g_k\|^2 \tag{1}$$

Cauchy point lies on boundary of the trust region $\Longrightarrow$

$$\alpha_k^{\mathrm{C}} = \frac{\Delta_k}{\|g_k\|}. \tag{2}$$

(1) + (2) $\Longrightarrow$

$$f_k - m_k(s_k^{\mathrm{C}}) \ge \|g_k\|^2 \frac{\Delta_k}{\|g_k\|} = \|g_k\|\Delta_k \ge \tfrac{1}{2}\|g_k\|\Delta_k.$$

Case (ii)

$$\alpha_k^* \stackrel{\text{def}}{=} \text{arg min } \; m_k(-\alpha g_k) \equiv f_k - \alpha\|g_k\|^2 + \tfrac{1}{2}\alpha^2 g_k^T B_k g_k \tag{3}$$

$\Longrightarrow$

$$\alpha_k^* = \frac{\|g_k\|^2}{g_k^T B_k g_k} \ge \alpha_k^{\mathrm{C}} = \frac{\Delta_k}{\|g_k\|} \tag{4}$$

$\Longrightarrow$

$$\alpha_k^{\mathrm{C}} g_k^T B_k g_k \le \|g_k\|^2. \tag{5}$$

(3) + (4) + (5) $\Longrightarrow$

$$\begin{aligned} f_k - m_k(s_k^{\mathrm{C}}) &= \alpha_k^{\mathrm{C}}\|g_k\|^2 - \tfrac{1}{2}[\alpha_k^{\mathrm{C}}]^2 g_k^T B_k g_k \ge \tfrac{1}{2}\alpha_k^{\mathrm{C}}\|g_k\|^2 \\ &= \tfrac{1}{2}\|g_k\|^2 \frac{\Delta_k}{\|g_k\|} = \tfrac{1}{2}\|g_k\|\Delta_k. \end{aligned}$$

Case (iii)

$$\alpha_k^{\mathrm{C}} = \alpha_k^* = \frac{\|g_k\|^2}{g_k^T B_k g_k}$$

$\Longrightarrow$

$$\begin{aligned} f_k - m_k(s_k^{\mathrm{C}}) &= \alpha_k^* \|g_k\|^2 + \tfrac{1}{2}(\alpha_k^*)^2 g_k^T B_k g_k \\ &= \frac{\|g_k\|^4}{g_k^T B_k g_k} - \tfrac{1}{2}\frac{\|g_k\|^4}{g_k^T B_k g_k} \\ &= \tfrac{1}{2}\frac{\|g_k\|^4}{g_k^T B_k g_k} \\ &\geq \tfrac{1}{2}\frac{\|g_k\|^2}{1 + \|B_k\|}, \end{aligned}$$

where

$$|g_k^T B_k g_k| \leq \|g_k\|^2 \|B_k\| \leq \|g_k\|^2 (1 + \|B_k\|)$$

because of the Cauchy-Schwarz inequality.

Corollary 3.2. If $m_k(s)$ is the second-order model, and s_k is an improvement on the Cauchy point within the trust-region $\|s\| \leq \Delta_k$,

$$f_k - m_k(s_k) \geq \tfrac{1}{2}\|g_k\| \min\left[\frac{\|g_k\|}{1 + \|B_k\|}, \Delta_k\right].$$

DIFFERENCE BETWEEN MODEL AND FUNCTION

Lemma 3.3. Suppose that $f \in C^2$, and that the true and model Hessians satisfy the bounds $\|H(x)\| \leq \kappa_h$ for all x and $\|B_k\| \leq \kappa_b$ for all k and some $\kappa_h \geq 1$ and $\kappa_b \geq 0$. Then

$$|f(x_k + s_k) - m_k(s_k)| \leq \kappa_d \Delta_k^2,$$

where $\kappa_d = \frac{1}{2}(\kappa_h + \kappa_b)$, for all k.

PROOF OF LEMMA 3.3

Mean value theorem $\Longrightarrow$

$$f(x_k + s_k) = f(x_k) + s_k^T \nabla_x f(x_k) + \tfrac{1}{2} s_k^T \nabla_{xx} f(\xi_k) s_k$$

for some $\xi_k \in [x_k, x_k + s_k]$. Thus

$$\begin{aligned} |f(x_k + s_k) - m_k(s_k)| &= \tfrac{1}{2}|s_k^T H(\xi_k) s_k - s_k^T B_k s_k| \leq \tfrac{1}{2}|s_k^T H(\xi_k) s_k| + \tfrac{1}{2}|s_k^T B_k s_k| \\ &\leq \tfrac{1}{2}(\kappa_h + \kappa_b)\|s_k\|^2 \leq \kappa_d \Delta_k^2 \end{aligned}$$

using the triangle and Cauchy-Schwarz inequalities.

ULTIMATE PROGRESS AT NON-OPTIMAL POINTS

Lemma 3.4. Suppose that $f \in C^2$, that the true and model Hessians satisfy the bounds $\|H_k\| \leq \kappa_h$ and $\|B_k\| \leq \kappa_b$ for all k and some $\kappa_h \geq 1$ and $\kappa_b \geq 0$, and that $\kappa_d = \frac{1}{2}(\kappa_h + \kappa_b)$. Suppose furthermore that $g_k \neq 0$ and that

$$\Delta_k \leq \|g_k\| \min\left(\frac{1}{\kappa_h + \kappa_b}, \frac{(1-\eta_v)}{2\kappa_d}\right).$$

Then iteration k is very successful and

$$\Delta_{k+1} \geq \Delta_k.$$

PROOF OF LEMMA 3.4

By definition,

$$1 + \|B_k\| \leq \kappa_h + \kappa_b$$

+ first bound on $\Delta_k \Longrightarrow$

$$\Delta_k \leq \frac{\|g_k\|}{\kappa_h + \kappa_b} \leq \frac{\|g_k\|}{1 + \|B_k\|}.$$

Corollary 3.2 $\Longrightarrow$

$$f_k - m_k(s_k) \geq \tfrac{1}{2}\|g_k\| \min\left[\frac{\|g_k\|}{1 + \|B_k\|}, \Delta_k\right] = \tfrac{1}{2}\|g_k\|\Delta_k.$$

+ Lemma 3.3 + second bound on $\Delta_k \Longrightarrow$

$$|\rho_k - 1| = \left|\frac{f(x_k + s_k) - m_k(s_k)}{f_k - m_k(s_k)}\right| \leq 2\frac{\kappa_d \Delta_k^2}{\|g_k\|\Delta_k} = 2\frac{\kappa_d \Delta_k}{\|g_k\|} \leq 1 - \eta_v.$$

$\Longrightarrow \rho_k \geq \eta_v \Longrightarrow$ iteration is very successful.

RADIUS WON'T SHRINK TO ZERO AT NON-OPTIMAL POINTS

Lemma 3.5. Suppose that $f \in C^2$, that the true and model Hessians satisfy the bounds $\|H_k\| \le \kappa_h$ and $\|B_k\| \le \kappa_b$ for all k and some $\kappa_h \ge 1$ and $\kappa_b \ge 0$, and that $\kappa_d = \frac{1}{2}(\kappa_h + \kappa_b)$. Suppose furthermore that there exists a constant $\epsilon > 0$ such that $\|g_k\| \ge \epsilon$ for all k. Then

$$\Delta_k \ge \kappa_\epsilon \stackrel{\text{def}}{=} \epsilon \gamma_d \min\left(\frac{1}{\kappa_h + \kappa_b}, \frac{(1-\eta_v)}{2\kappa_d}\right)$$

for all k.

PROOF OF LEMMA 3.5

Suppose otherwise that iteration k is first for which

$$\Delta_{k+1} \le \kappa_\epsilon.$$

$\Delta_k > \Delta_{k+1} \implies$ iteration k unsuccessful $\implies \gamma_d \Delta_k \le \Delta_{k+1}$. Hence

$$\begin{aligned}\Delta_k &\le \epsilon \min\left(\frac{1}{\kappa_h + \kappa_b}, \frac{(1-\eta_v)}{2\kappa_d}\right) \\ &\le \|g_k\| \min\left(\frac{1}{\kappa_h + \kappa_b}, \frac{(1-\eta_v)}{2\kappa_d}\right)\end{aligned}$$

But this contradicts assertion of Lemma 3.4 that iteration k must be very successful.

POSSIBLE FINITE TERMINATION

Lemma 3.6. Suppose that $f \in C^2$, and that both the true and model Hessians remain bounded for all k. Suppose furthermore that there are only finitely many successful iterations. Then $x_k = x_*$ for all sufficiently large k and $g(x_*) = 0$.

PROOF OF LEMMA 3.6

$$x_{k_0+j} = x_{k_0+1} = x_*$$

for all $j > 0$, where k_0 is index of last successful iterate.

All iterations are unsuccessful for sufficiently large $k \Longrightarrow \{\Delta_k\} \longrightarrow 0$

\+ Lemma 3.4 then implies that if $\|g_{k_0+1}\| > 0$ there must be a successful iteration of index larger than k_0, which is impossible $\Longrightarrow \|g_{k_0+1}\| = 0$.

GLOBAL CONVERGENCE OF ONE SEQUENCE

Theorem 3.7. Suppose that $f \in C^2$, and that both the true and model Hessians remain bounded for all k. Then either

$$g_l = 0 \ \text{ for some } \ l \geq 0$$

or

$$\lim_{k \to \infty} f_k = -\infty$$

or

$$\liminf_{k \to \infty} \|g_k\| = 0.$$

PROOF OF THEOREM 3.7

Let $\mathcal{S}$ be the index set of successful iterations. Lemma 3.6 $\Longrightarrow$ true Theorem 3.7 when $|\mathcal{S}|$ finite.

So consider $|\mathcal{S}| = \infty$, and suppose f_k bounded below and

$$\|g_k\| \geq \epsilon \tag{6}$$

for some $\epsilon > 0$ and all k, and consider some $k \in \mathcal{S}$.

+ Corollary 3.2, Lemma 3.5, and the assumption (6) $\Longrightarrow$

$$f_k - f_{k+1} \geq \eta_s[f_k - m_k(s_k)] \geq \delta_\epsilon \stackrel{\text{def}}{=} \tfrac{1}{2}\eta_s \epsilon \min\left[\frac{\epsilon}{1+\kappa_b}, \kappa_\epsilon\right].$$

$\Longrightarrow$

$$f_0 - f_{k+1} = \sum_{\substack{j=0 \\ j \in \mathcal{S}}}^{k} [f_j - f_{j+1}] \geq \sigma_k \delta_\epsilon,$$

where σ_k is the number of successful iterations up to iteration k. But

$$\lim_{k \to \infty} \sigma_k = +\infty.$$

$\Longrightarrow$ f_k unbounded below $\Longrightarrow$ a subsequence of the $\|g_k\| \longrightarrow 0$

GLOBAL CONVERGENCE

Theorem 3.8. Suppose that $f \in C^2$, and that both the true and model Hessians remain bounded for all k. Then either

$$g_l = 0 \text{ for some } l \geq 0$$

or

$$\lim_{k \to \infty} f_k = -\infty$$

or

$$\lim_{k \to \infty} g_k = 0.$$

PROOF OF THEOREM 3.8

Suppose otherwise that f_k is bounded from below, and that there is a subsequence $\{t_i\} \subseteq \mathcal{S}$, such that

$$\|g_{t_i}\| \geq 2\epsilon > 0 \tag{7}$$

for some $\epsilon > 0$ and for all i. Theorem 3.7 $\Longrightarrow$ $\exists \{\ell_i\} \subseteq \mathcal{S}$ such that

$$\|g_k\| \geq \epsilon \text{ for } t_i \leq k < \ell_i \text{ and } \|g_{\ell_i}\| < \epsilon. \tag{8}$$

Now restrict attention to indices in

$$\mathcal{K} \stackrel{\text{def}}{=} \{k \in \mathcal{S} \mid t_i \leq k < \ell_i\}.$$

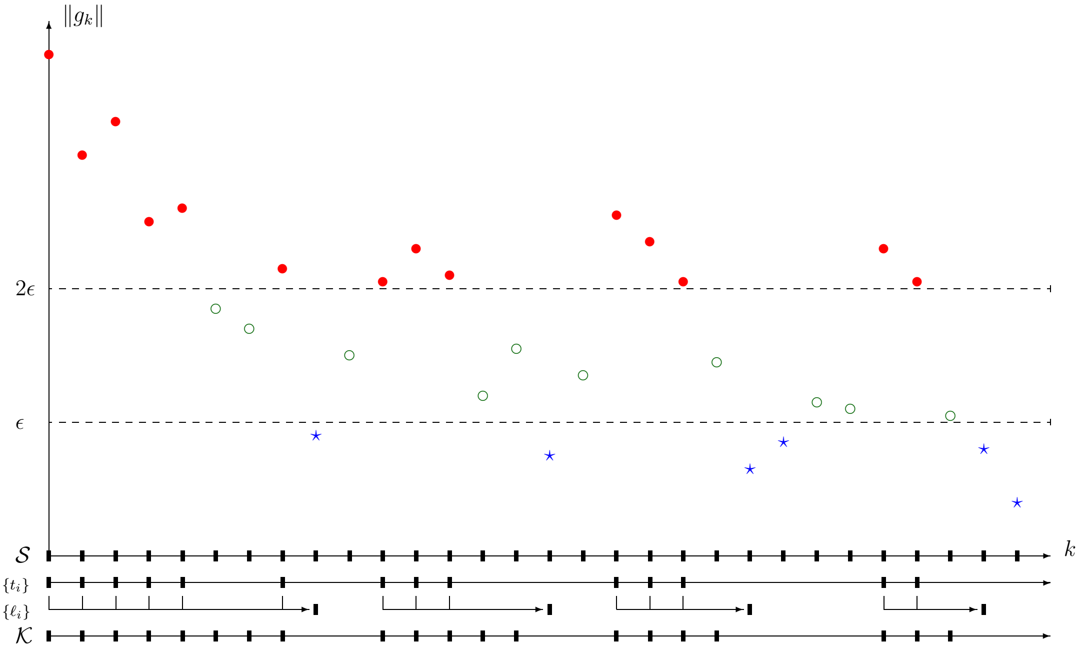


Figure 3.1: The subsequences of the proof of Theorem 3.8

As in proof of Theorem 3.7, (8) $\Longrightarrow$

$$f_k - f_{k+1} \geq \eta_s[f_k - m_k(s_k)] \geq \tfrac{1}{2}\eta_s\epsilon \min\left[\frac{\epsilon}{1+\kappa_b}, \Delta_k\right] \tag{9}$$

for all $k \in \mathcal{K} \Longrightarrow$ LHS of (9) $\longrightarrow 0$ as $k \longrightarrow \infty \Longrightarrow$

$$\lim_{\substack{k\to\infty \\ k\in\mathcal{K}}} \Delta_k = 0$$

$\Longrightarrow$

$$\Delta_k \leq \frac{2}{\epsilon\eta_s}[f_k - f_{k+1}].$$

for $k \in \mathcal{K}$ sufficiently large $\Longrightarrow$

$$\|x_{t_i} - x_{\ell_i}\| \leq \sum_{\substack{j=t_i \\ j\in\mathcal{K}}}^{\ell_i-1} \|x_j - x_{j+1}\| \leq \sum_{\substack{j=t_i \\ j\in\mathcal{K}}}^{\ell_i-1} \Delta_j \leq \frac{2}{\epsilon\eta_s}[f_{t_i} - f_{\ell_i}]. \tag{10}$$

for i sufficiently large.

But RHS of (10) $\longrightarrow 0 \Longrightarrow \|x_{t_i} - x_{\ell_i}\| \longrightarrow 0$ as i tends to infinity + continuity $\Longrightarrow \|g_{t_i} - g_{\ell_i}\| \longrightarrow 0$.

Impossible as $\|g_{t_i} - g_{\ell_i}\| \geq \epsilon$ by definition of $\{t_i\}$ and $\{\ell_i\}$ $\Longrightarrow$ no subsequence satisfying (7) can exist.

II: SOLVING THE TRUST-REGION SUBPROBLEM

$$\text{(approximately) } \underset{s \in \mathbb{R}^n}{\text{minimize}} \;\; q(s) \equiv s^T g + \tfrac{1}{2} s^T B s \;\; \text{subject to} \;\; \|s\| \leq \Delta$$

AIM: find s_* so that

$$q(s_*) \leq q(s^{\mathrm{C}}) \;\; \text{and} \;\; \|s_*\| \leq \Delta$$

Might solve

- $\odot$ exactly $\Longrightarrow$ Newton-like method
- $\odot$ approximately $\Longrightarrow$ steepest descent/conjugate gradients

THE ℓ_2-NORM TRUST-REGION SUBPROBLEM

$$\underset{s \in \mathbb{R}^n}{\text{minimize}} \;\; q(s) \equiv s^T g + \tfrac{1}{2} s^T B s \;\; \text{subject to} \;\; \|s\|_2 \leq \Delta$$

Solution characterisation result:

Theorem 3.9. Any *global* minimizer s_* of $q(s)$ subject to $\|s\|_2 \leq \Delta$ satisfies the equation

$$(B + \lambda_* I) s_* = -g,$$

where $B + \lambda_* I$ is positive semi-definite, $\lambda_* \geq 0$ and $\lambda_*(\|s_*\|_2 - \Delta) = 0$. If $B + \lambda_* I$ is positive definite, s_* is unique.

PROOF OF THEOREM 3.9

Problem equivalent to minimizing $q(s)$ subject to $\frac{1}{2}\Delta^2 - \frac{1}{2}s^T s \geq 0$. Theorem 1.9 $\Longrightarrow$

$$g + B s_* = -\lambda_* s_* \tag{11}$$

for some Lagrange multiplier $\lambda_* \geq 0$ for which either $\lambda_* = 0$ or $\|s_*\|_2 = \Delta$ (or both). It remains to show $B + \lambda_* I$ is positive semi-definite.

If s_* lies in the interior of the trust-region, $\lambda_* = 0$, and Theorem 1.10 $\Longrightarrow$ $B + \lambda_* I = B$ is positive semi-definite.

If $\|s_*\|_2 = \Delta$ and $\lambda_* = 0$, Theorem 1.10 $\Longrightarrow$ $v^T B v \geq 0$ for all $v \in \mathcal{N}_+ = \{v | s_*^T v \geq 0\}$. If $v \notin \mathcal{N}_+ \Longrightarrow -v \in \mathcal{N}_+ \Longrightarrow v^T B v \geq 0$ for all v.

Only remaining case is where $\|s_*\|_2 = \Delta$ and $\lambda_* > 0$. Theorem 1.10 $\Longrightarrow$ $v^T(B + \lambda_* I)v \geq 0$ for all $v \in \mathcal{N}_+ = \{v | s_*^T v = 0\}$ $\Longrightarrow$ remains to consider $v^T B v$ when $s_*^T v \neq 0$.

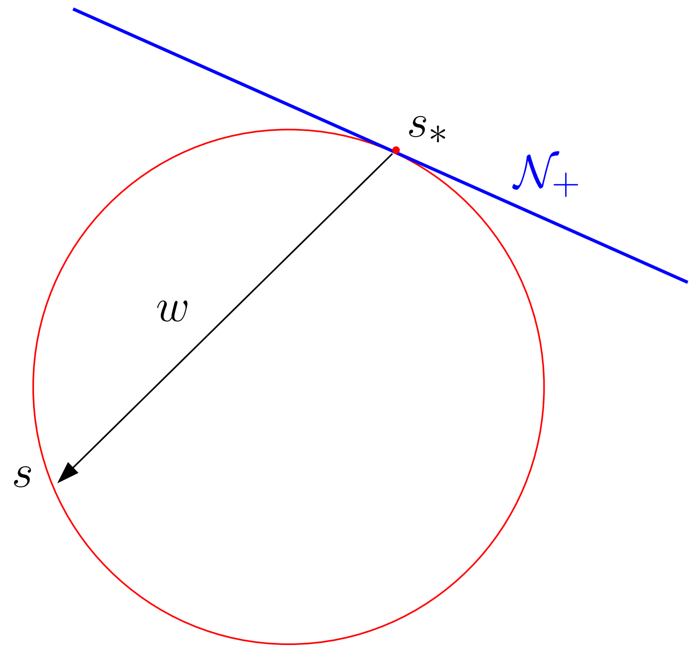


Figure 3.2: Construction of "missing" directions of positive curvature.

Let s be any point on the boundary δR of the trust-region R, and let $w = s - s_*$. Then

$$-w^T s_* = (s_* - s)^T s_* = \tfrac{1}{2}(s_* - s)^T (s_* - s) = \tfrac{1}{2} w^T w \qquad (12)$$

since $\|s\|_2 = \Delta = \|s_*\|_2$. (11) + (12) $\Longrightarrow$

$$\begin{aligned} q(s) - q(s_*) &= w^T(g + Bs_*) + \tfrac{1}{2} w^T B w \\ &= -\lambda_* w^T s_* + \tfrac{1}{2} w^T B w = \tfrac{1}{2} w^T (B + \lambda_* I) w, \end{aligned} \qquad (13)$$

$\Longrightarrow$ $w^T(B + \lambda_* I)w \geq 0$ since s_* is a global minimizer. But

$$s = s_* - 2\frac{s_*^T v}{v^T v} v \in \delta R$$

$\Longrightarrow$ (for this s) $w \| v \Longrightarrow v^T(B + \lambda_* I)v \geq 0$.

When $B + \lambda_* I$ is positive definite, $s_* = -(B + \lambda_* I)^{-1} g$. If $s_* \in \delta R$ and $s \in R$, (12) and (13) become $-w^T s_* \geq \frac{1}{2} w^T w$ and $q(s) \geq q(s_*) + \frac{1}{2} w^T (B + \lambda_* I) w$ respectively. Hence, $q(s) > q(s_*)$ for any $s \neq s_*$. If s_* is interior, $\lambda_* = 0$, B is positive definite, and thus s_* is the unique unconstrained minimizer of $q(s)$.

ALGORITHMS FOR THE ℓ_2-NORM SUBPROBLEM

Two cases:

- ⊙ B positive-semi definite and $Bs = -g$ satisfies $\|s\|_2 \leq \Delta \Longrightarrow s_* = s$
- ⊙ B indefinite or $Bs = -g$ satisfies $\|s\|_2 > \Delta$
  In this case
  - ⋄ $(B + \lambda_* I)s_* = -g$ and $s_*^T s_* = \Delta^2$
  - ⋄ nonlinear (quadratic) system in s and λ
  - ⋄ concentrate on this

EQUALITY CONSTRAINED ℓ_2-NORM SUBPROBLEM

Suppose B has spectral decomposition

$$B = U^T \Lambda U$$

- ⊙ U eigenvectors
- ⊙ Λ diagonal eigenvalues: $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$

Require $B + \lambda I$ positive semi-definite $\Longrightarrow \lambda \geq -\lambda_1$

Define

$$s(\lambda) = -(B + \lambda I)^{-1} g$$

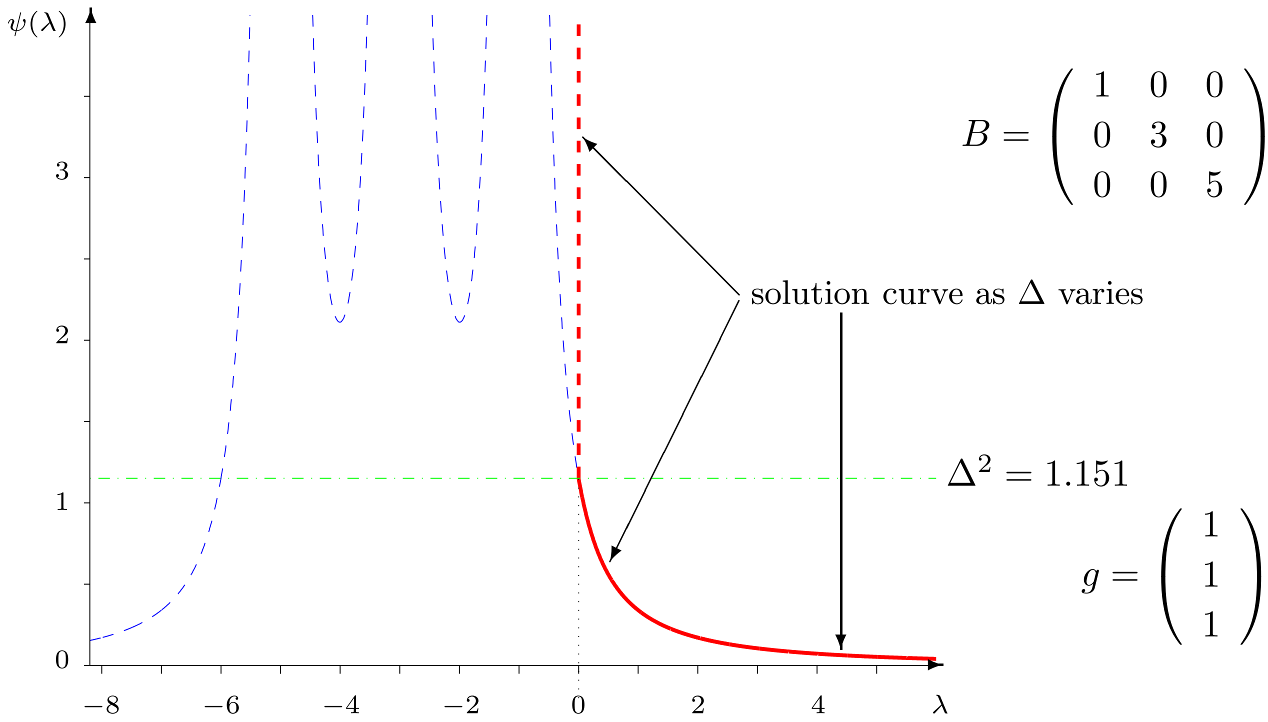
Require

$$\psi(\lambda) \stackrel{\text{def}}{=} \|s(\lambda)\|_2^2 = \Delta^2$$

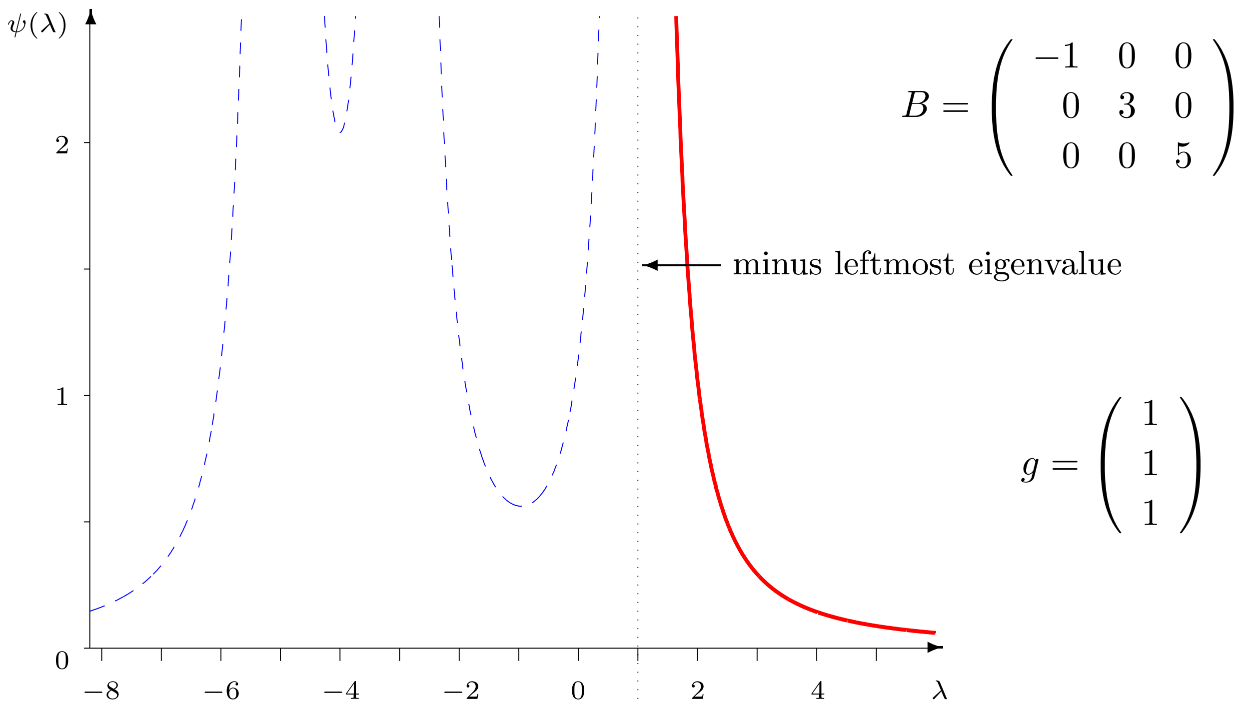
Note $(\gamma_i = e_i^T U g)$

$$\psi(\lambda) = \|U^T (\Lambda + \lambda I)^{-1} U g\|_2^2 = \sum_{i=1}^{n} \frac{\gamma_i^2}{(\lambda_i + \lambda)^2}$$

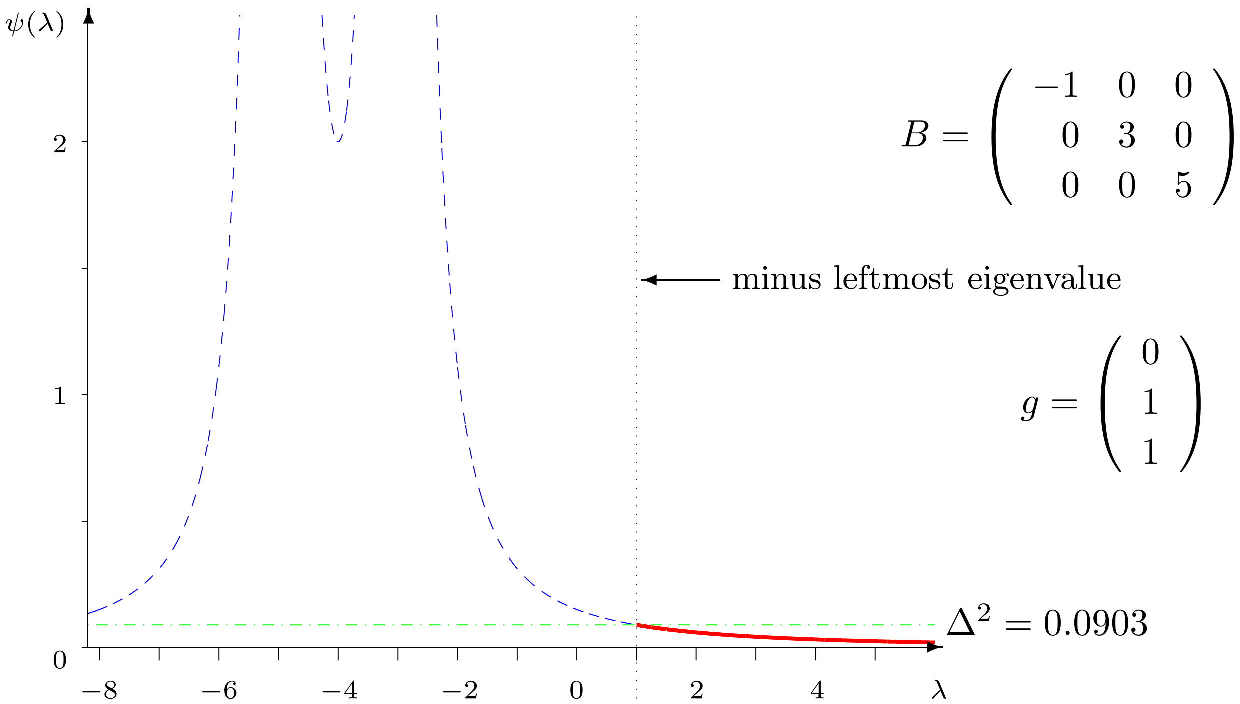
CONVEX EXAMPLE



NONCONVEX EXAMPLE



THE “HARD” CASE



SUMMARY

For indefinite B,

Hard case occurs when g orthogonal to eigenvector u_1 for most negative eigenvalue λ_1

- OK if radius is radius small enough
- No “obvious” solution to equations . . . but solution is actually of the form

$$s_{\text{lim}} + \sigma u_1$$

where

- $s_{\text{lim}} = \lim_{\lambda \xrightarrow{+} -\lambda_1} s(\lambda)$
- $\|s_{\text{lim}} + \sigma u_1\|_2 = \Delta$

HOW TO SOLVE $\|\mathbf{s}(\lambda)\|_2 = \Delta$

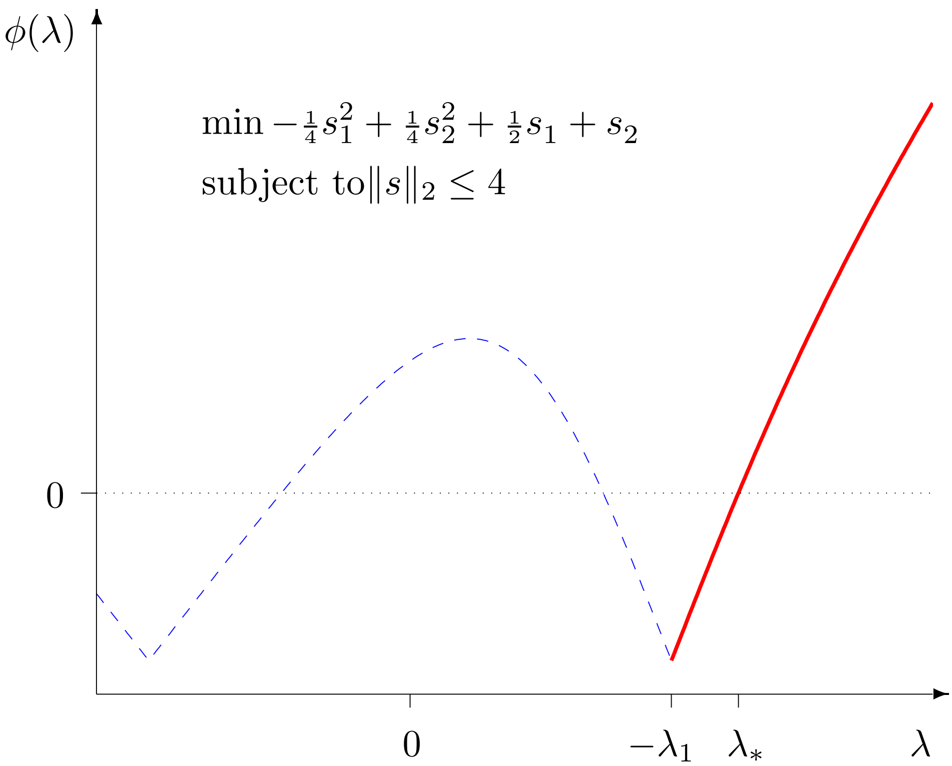
DON'T!!

Solve instead the **secular equation**

$$\phi(\lambda) \stackrel{\text{def}}{=} \frac{1}{\|s(\lambda)\|_2} - \frac{1}{\Delta} = 0$$

- ⊙ no poles
- ⊙ smallest at eigenvalues (except in hard case!)
- ⊙ analytic function $\Longrightarrow$ ideal for Newton
- ⊙ global convergent (ultimately quadratic rate except in hard case)
- ⊙ need to safeguard to protect Newton from the hard & interior solution cases

THE SECULAR EQUATION



NEWTON'S METHOD FOR SECULAR EQUATION

Newton correction at λ is $-\phi(\lambda)/\phi'(\lambda)$. Differentiating

$$\phi(\lambda) = \frac{1}{\|s(\lambda)\|_2} - \frac{1}{\Delta} = \frac{1}{(s^T(\lambda)s(\lambda))^{\frac{1}{2}}} - \frac{1}{\Delta} \implies$$

$$\phi'(\lambda) = -\frac{s^T(\lambda)\nabla_\lambda s(\lambda)}{(s^T(\lambda)s(\lambda))^{\frac{3}{2}}} = -\frac{s^T(\lambda)\nabla_\lambda s(\lambda)}{\|s(\lambda)\|_2^3}.$$

Differentiating the defining equation

$$(B+\lambda I)s(\lambda) = -g \implies (B+\lambda I)\nabla_\lambda s(\lambda) + s(\lambda) = 0.$$

Notice that, rather than $\nabla_\lambda s(\lambda)$, merely

$$s^T(\lambda)\nabla_\lambda s(\lambda) = -s^T(\lambda)(B+\lambda I)(\lambda)^{-1}s(\lambda)$$

required for $\phi'(\lambda)$. Given the factorization $B+\lambda I = L(\lambda)L^T(\lambda) \implies$

$$\begin{aligned} s^T(\lambda)(B+\lambda I)^{-1}s(\lambda) &= s^T(\lambda)L^{-T}(\lambda)L^{-1}(\lambda)s(\lambda) \\ &= (L^{-1}(\lambda)s(\lambda))^T(L^{-1}(\lambda)s(\lambda)) = \|w(\lambda)\|_2^2 \end{aligned}$$

where $L(\lambda)w(\lambda) = s(\lambda)$.

NEWTON'S METHOD & THE SECULAR EQUATION

Let $\lambda > -\lambda_1$ and $\Delta > 0$ be given
Until "convergence" do:
  Factorize $B+\lambda I = LL^T$
  Solve $LL^Ts = -g$
  Solve $Lw = s$
  Replace λ by

$$\lambda + \left(\frac{\|s\|_2 - \Delta}{\Delta}\right)\left(\frac{\|s\|_2^2}{\|w\|_2^2}\right)$$

SOLVING THE LARGE-SCALE PROBLEM

- when n is large, factorization may be impossible
- may instead try to use an iterative method to approximate
  - Steepest descent leads to the Cauchy point
  - obvious generalization: conjugate gradients … but
    - what about the trust region?
    - what about negative curvature?

CONJUGATE GRADIENTS TO "MINIMIZE" q(s)

Given $s^0 = 0$, set $g^0 = g$, $d^0 = -g$ and $i = 0$
Until g^i "small" or breakdown, iterate

$$\alpha^i = \|g^i\|_2^2 / d^{i\,T} B d^i$$
$$s^{i+1} = s^i + \alpha^i d^i$$
$$g^{i+1} = g^i + \alpha^i B d^i$$
$$\beta^i = \|g^{i+1}\|_2^2 / \|g^i\|_2^2$$
$$d^{i+1} = -g^{i+1} + \beta^i d^i$$

and increase i by 1

Important features

- $g^j = Bs^j + g$ for all $j = 0, \ldots, i$
- $d^{j\,T} g^{i+1} = 0$ for all $j = 0, \ldots, i$
- $g^{j\,T} g^{i+1} = 0$ for all $j = 0, \ldots, i$

CRUCIAL PROPERTY OF CONJUGATE GRADIENTS

Theorem 3.10. Suppose that the conjugate gradient method is applied to minimize $q(s)$ starting from $s^0 = 0$, and that $d^{i\,T} B d^i > 0$ for $0 \leq i \leq k$. Then the iterates s^j satisfy the inequalities

$$\|s^j\|_2 < \|s^{j+1}\|_2$$

for $0 \leq j \leq k-1$.

PROOF OF THEOREM 3.10

First show that

$$d^{i\,T} d^j = \frac{\|g^i\|_2^2}{\|g^j\|_2^2} \|d^j\|_2^2 > 0 \qquad (14)$$

for all $0 \leq j \leq i \leq k$. For any i, (14) is trivially true for $j = i$. Suppose it is also true for all $i \leq l$. Then, the update for d^{l+1} gives

$$d^{l+1} = -g^{l+1} + \frac{\|g^{l+1}\|_2^2}{\|g^l\|_2^2} d^l.$$

Forming the inner product with d^j, and using the fact that $d^{j\,T} g^{l+1} = 0$ for all $j = 0, \ldots, l$, and (14) when $j = l$, reveals

$$\begin{aligned} d^{l+1\,T} d^j &= -g^{l+1\,T} d^j + \frac{\|g^{l+1}\|_2^2}{\|g^l\|_2^2} d^{l\,T} d^j \\ &= \frac{\|g^{l+1}\|_2^2}{\|g^l\|_2^2} \frac{\|g^l\|_2^2}{\|g^j\|_2^2} \|d^j\|_2^2 = \frac{\|g^{l+1}\|_2^2}{\|g^j\|_2^2} \|d^j\|_2^2 > 0. \end{aligned}$$

Thus (14) is true for $i \leq l+1$, and hence for all $0 \leq j \leq i \leq k$.

Now have from the algorithm that

$$s^i = s^0 + \sum_{j=0}^{i-1} \alpha^j d^j = \sum_{j=0}^{i-1} \alpha^j d^j$$

as, by assumption, $s^0 = 0$. Hence

$$s^{i\,T} d^i = \sum_{j=0}^{i-1} \alpha^j d^{j\,T} d^i = \sum_{j=0}^{i-1} \alpha^j d^{j\,T} d^i > 0 \tag{15}$$

as each $\alpha^j > 0$, which follows from the definition of α^j, since $d^{j\,T} H d^j > 0$, and from relationship (14). Hence

$$\begin{aligned} \|s^{i+1}\|_2^2 &= s^{i+1\,T} s^{i+1} = \left(s^i + \alpha^i d^i\right)^T \left(s^i + \alpha^i d^i\right) \\ &= s^{i\,T} s^i + 2\alpha^i s^{i\,T} d^i + \alpha^{i\,2} d^{i\,T} d^i > s^{i\,T} s^i = \|s^i\|_2^2 \end{aligned}$$

follows directly from (15) and $\alpha^i > 0$ which is the required result.

TRUNCATED CONJUGATE GRADIENTS

Apply the conjugate gradient method, but terminate at iteration i if

1. $d^{i\,T} B d^i \leq 0 \Longrightarrow$ problem unbounded along d^i
2. $\|s^i + \alpha^i d^i\|_2 > \Delta \Longrightarrow$ solution on trust-region boundary

In both cases, stop with $s_* = s^i + \alpha^{\mathrm{B}} d^i$, where α^{B} chosen as positive root of

$$\|s^i + \alpha^{\mathrm{B}} d^i\|_2 = \Delta$$

Crucially

$$q(s_*) \leq q(s^{\mathrm{C}}) \ \text{ and } \ \|s_*\|_2 \leq \Delta$$

$\Longrightarrow$ TR algorithm converges to a first-order critical point

HOW GOOD IS TRUNCATED C.G.?

In the convex case . . . very good

Theorem 3.11. Suppose that the truncated conjugate gradient method is applied to minimize $q(s)$ and that B is positive definite. Then the computed and actual solutions to the problem, s_* and s_*^{M}, satisfy the bound

$$q(s_*) \leq \tfrac{1}{2} q(s_*^{\mathrm{M}})$$

In the non-convex case . . . maybe poor

- e.g., if $g = 0$ and B is indefinite $\Longrightarrow$ $q(s_*) = 0$

WHAT CAN WE DO IN THE NON-CONVEX CASE?

Solve the problem over a subspace

- instead of the B-conjugate subspace for CG, use the equivalent Lanczos orthogonal basis
  - Gram-Schmidt applied to CG (Krylov) basis $\mathcal{D}^i$
  - Subspace $\mathcal{Q}^i = \{s \mid s = Q^i s_q \text{ for some } s_q \in \mathrm{IR}^i\}$
  - Q^i is such that

    $$Q^{i\,T} Q^i = I \text{ and } Q^{i\,T} B Q^i = T^i$$

    where T^i is tridiagonal and $Q^{i\,T} g = \|g\|_2 \, e_1$
  - Q^i trivial to generate from CG $\mathcal{D}^i$

GENERALIZED LANCZOS TRUST-REGION METHOD

$$s^i = \arg\min_{s \in \mathcal{Q}^i} q(s) \ \text{ subject to } \ \|s\|_2 \leq \Delta$$

$\Longrightarrow$ $s^i = Q^i s^i_q$, where

$$s^i_q = \arg\min_{s_q \in \mathrm{I\!R}^i} \|g\|_2 \, e_1^T s_q + \tfrac{1}{2} s_q^T T^i s_q \ \text{ subject to } \ \|s_q\|_2 \leq \Delta$$

- ⊙ advantage T^i has very sparse factors $\Longrightarrow$ can solve the problem using the earlier secular equation approach
- ⊙ can exploit all the structure here $\Longrightarrow$ use solution for one problem to initialize next
- ⊙ until the trust-region boundary is reached, it **is** conjugate gradients $\Longrightarrow$ switch when we get there