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Exercise 7 - Solution

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Homework Problem 7.1 (Trust-Region Subproblem Solutions for varying Δ) 6 Points

Consider the trust region subproblems

$$\begin{aligned} &\text{Minimize} \quad q(s) = f(x) + f'(x)\, s + \frac{1}{2}\, s^\intercal H s, \quad \text{where } s \in \mathbb{R}^n \\ &\text{subject to} \quad \|s\|_M \le \Delta \end{aligned} \tag{6.1}$$

for $f \in \mathbb{C}^2$, a symmetric model Hessian $H \in \mathbb{R}^{n\times n}$, a Norm induced by the s. p. d. $M \in \mathbb{R}^{n\times n}$ and $\Delta > 0$ with the corresponding Δ family of subproblem solutions

$$S_{\bar{\Delta}} := \{s \in \mathbb{R}^n \mid s \text{ solves (6.1) for } \Delta \in [0, \bar{\Delta}]\}$$

and the corresponding necessary and sufficient optimality systems

$$\mu \ge 0, \quad \|s\|_M - \Delta \le 0, \quad \mu\,(\|s\|_M - \Delta) = 0 \tag{6.18a}$$

$$(H + \mu\, M)\, s = -f'(x)^\intercal \tag{6.18b}$$

$$H + \mu\, M \text{ is positive semidefinite} \tag{6.18c}$$

for $s \in \mathbb{R}^n$ and unique $\mu \in \mathbb{R}$.

(i) Derive a characterization for the solution s of (6.1) and the corresponding μ depending on Δ for the case where $H = M$ and interpret the result in terms of $S_{\bar{\Delta}}$.

(ii) Use (6.18) to create a visualization of S_2 for Rosenbrock's function for $M = \mathrm{Id}$, both choices of $x \in \{(0, -1)^\intercal, (0, 0.5)^\intercal\}$ and for both $H = \mathrm{Id}$ and $H = f''(x)$.

Solution.

(i) When $H = M$, then both matrices are s. p. d., so the trust-region subproblems are convex with strictly convex cost functional and hence they are uniquely solvable, meaning that both s and μ are unique.

In fact, independent of μ, the matrix

$$H + \mu M = (1 + \mu)M$$

is even s. p. d. instead of only semidefinite. Its inverse is given by

$$(H + \mu M)^{-1} = \frac{1}{1+\mu} M^{-1}$$

so that

$$s = -\frac{1}{1+\mu} M^{-1} f'(x)^\intercal = -\frac{1}{1+\mu} \nabla_M f(x). \tag{0.2}$$

From (6.18a) we can gather that either $\mu = 0$ and $\|\nabla_M f(x)\|_M < \Delta$ or

$$\Delta = \|s\|_M = \frac{1}{1+\mu} \|\nabla_M f(x)\|_M \Rightarrow \mu = \frac{\|\nabla_M f(x)\|_M}{\Delta} - 1$$

so that

$$\mu = \begin{cases} 0 & \|\nabla_M f(x)\|_M < \Delta \\ \frac{\|\nabla_M f(x)\|_M}{\Delta} - 1 & \|\nabla_M f(x)\|_M \geq \Delta \end{cases}. \tag{0.3}$$

Equations (0.2) and (0.3) fully characterize the solutions to the trust region subproblems. They show that when the model is strongly convex with the same curvature information as the bounding constraint, then the solutions depending on Δ are simply scaled versions of the M/H gradient that is shortened to stay within the bounding ball if necessary. The Δ family $S_{\bar{\Delta}}$ is therefore simply a line segment that is either cut short if $\bar{\Delta} < \|\nabla_M f(x)\|_M$ or ends at $\nabla_M f(x)$.

Generally, when the subproblem is uniquely solvable, the $S_{\bar{\Delta}}$ will be a path segment with curvature that is dependent on the interaction of H and M but μ still plays the role of a scaling parameter in the solution of (6.18b).

(ii) In the case of $H = M = \mathrm{Id}$, we already know we should expect scaled euclidean gradients with nonlinear scaling with respect to μ and linear scaling with respect to Δ, which can be seen in **??**

Otherwise, Equation (6.18b) is equivalent to

$$\underbrace{Hs + f'(x)}_{q'(s)} = -\mu \underbrace{Ms}_{\frac{\partial}{\partial s}\frac{1}{2}(\|s\|_M^2 - \Delta^2)}$$

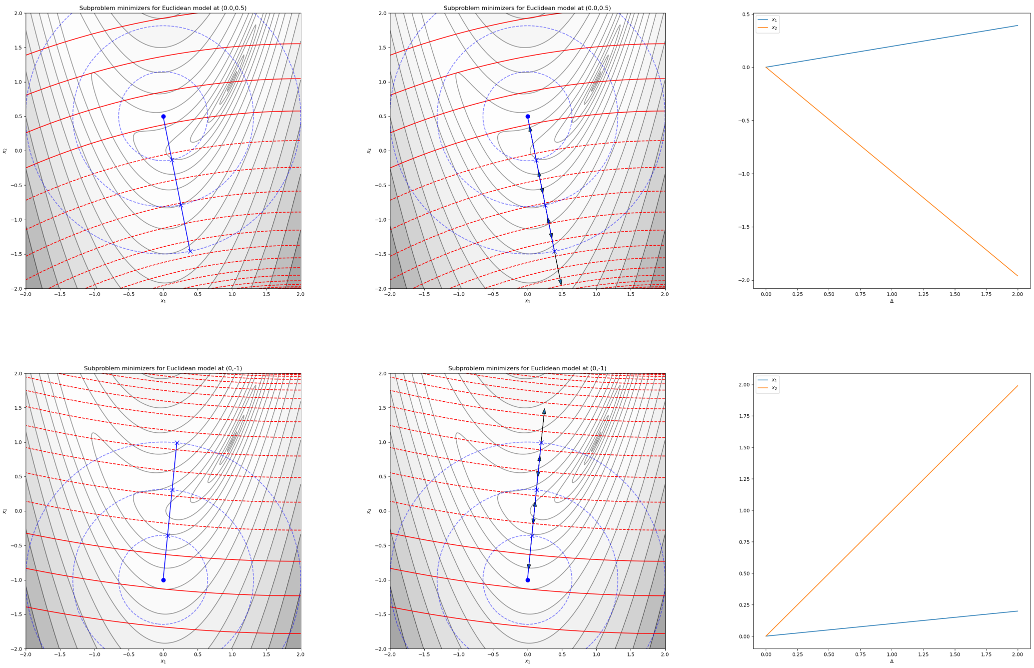

Figure 0.1: Isolines of Rosenbrock function (gray), Euclidean quadratic models shifted to x (red) and trust region bound constraint functions (blue) for Rosenbrock's function (left), same plot with some normalized gradients of model and constraint along the minimizers (middle) and location of the respective minimizers with varying Δ (right) for points $x = (0, -1)$ and $(x = (0, 0.5)$ (top to bottom).

meaning that the solutions are either stationary points of the quadratic model with $\mu = 0$ or they lie on the boundary of the trust region with $\mu > 0$ and the euclidean gradients (normals of the isolines) of the ball constraint and the quadratic model are antiparallel. (This also applies to the case $H = M = \mathrm{Id}$ of course.)

When H is the Hessian at x, we have the following data for Rosenbrock's function with $a, b \geq 1$

$$\begin{aligned} f(x_1, x_2) &= (a - x_1)^2 + b(x_2 - x_1^2)^2 \\ f'(x_1, x_2) &= (-2\,(a - x_1) - 4bx_1\,(x_2 - x_1^2), \quad 2b\,(x_2 - x_1^2)) \\ f''(x_1, x_2) &= \begin{pmatrix} 2 - 4b\,(x_2 - 3x_1^2) & -4bx_1 \\ -4bx_1 & 2b \end{pmatrix} \end{aligned}$$

I. e., at $(0, -1)$ and $(0, 0.5)$, we have

$$\begin{aligned} f(0, -1) &= a^2 + b & f(0, 0.5) &= a^2 + b/4 \\ f'(0, -1) &= (-2a, \quad -2b) & f'(0, 0.5) &= (-2a, \quad b) \\ f''(0, -1) &= \begin{pmatrix} 2 + 4b & 0 \\ 0 & 2b \end{pmatrix} & f''(0, 0.5) &= \begin{pmatrix} 2 - 2b & 0 \\ 0 & 2b \end{pmatrix}. \end{aligned}$$

In both cases, the hessians are diagonal and (except for the case where $b = 1$, which we exclude from this investigation) they are nonsingular but don't conincide with the identiy. The hessian at $(0, -1)$ is s. p. d. while the hessian at $(0, 0.5)$ is indefinite. For any Δ, the quadratic model in the case of $x = (0, -1)$ is therefore strongly convex and has a unique global minimizer which is the only stationary point. The model for $x = (0, 0.5)$ is indefinite and only has a single stationary point which is a saddle point.

For $M = \mathrm{Id}$ and any diagonal matrix H

$$H = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

(6.18c) implies that $\mu \geq \max(-\lambda_1, -\lambda_2, 0)$. Meaning that μ can only be 0 if all $\lambda_i > 0$ (i. e. when H is s. p. d. to begin with). When H is not s. p. d. but indefinite, like in the case of H being the hessian $f''(0, 0.5)$, where we have a direction of negative curvature, we know that $\mu > 0$, meaning s always lies on the boundary of the trust region (this is expected when negative curvature is present).

For $x = (0, -1)$ we can therefore simply proceed to plot the isolines of the quadratic model and the ball constraint, check for stationary points inside the largest trust region ball and follow them along paths where the constraint and isoline normals are antiparallel. If the largest trust region

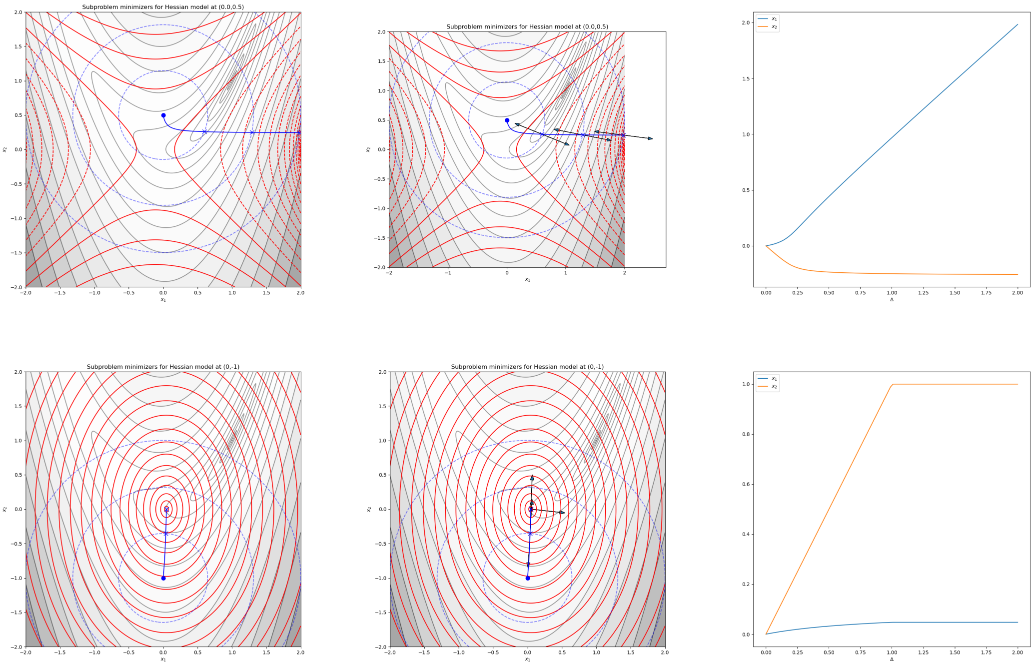

Figure 0.2: Isolines of Rosenbrock function (gray), full quadratic models shifted to x (red) and trust region bound constraint functions (blue) for Rosenbrock's function (left), same plot with some normalized gradients of model and constraint along the minimizers (middle) and location of the respective minimizers with varying Δ (right) for points $x = (0, -1)$ and $(x = (0, 0.5)$ (top to bottom).

does not contain a stationary point, we proceed as for $x = (0, 0.5)$, where we already know that for any trust region ball, the solution is on the boundary and the geadients are antiparallel.

Figure 0.2 shows the expected behavior of the subproblem solutions and the gradients. Note that the gradients in the bottom row (middle image) are showing numerical defects because the minimizer is a stationary point with numerically almost vanishing gradients. Additionally, on the bottom row $x = (0, -1)$ we can nicely observe that the local minimizer remains constant until Δ is sufficiently small.

(6 Points)

Homework Problem 7.2 (Saving a Function Evaluation per Trust-Region-Iteration) 3 Points

Remark 6.2 states that the quadratic model evaluation in the generic trust-region-Algorithm 6.1 is "typically a by-product of the solution of the trust-region subproblem (6.1)". Explain how the Steihaug-Toint-CG (Algorithm 6.14) has to be modified to be able to return this value for only three additional floating point operations per successfull CG iteration (plus minor additional work for initialization and termination).

Solution.

As shown in (4.8) of the lecture notes, the update to the function value of a quadratic function

$$q(s) = f - b^\top s + \frac{1}{2}\, s^\top H\, s$$

for a conjugate gradient update step $s \longrightarrow s + \alpha p$ is given by

$$\begin{aligned} q(s + \alpha\, p) - q(s) &= \frac{1}{2}(s + \alpha\, p)^\top H\, (s + \alpha\, p) - b^\top (s + \alpha\, p) + c - \frac{1}{2} s^\top H\, s + b^\top s - c \\ &= \frac{1}{2}(p^\top H\, p)\, \alpha^2 + (H\, s - b)^\top p\, \alpha \\ &= \frac{1}{2}\, \underbrace{(p^\top H\, p)}_{\theta}\, \alpha^2 + \underbrace{(\zeta^\top p)}_{-\delta}\, \alpha \\ &= \alpha(\frac{1}{2}\alpha\theta - \delta), \end{aligned}$$

where $\zeta^\top p = \delta$ holds because the residual ζ is orthogonal to all previous directions.

Evaluating this expression when θ and δ have previously been computed requires 4 floating point operations (so 5 floating point operations is the amount of work needed to update the previous iterate's function value when the Steihaug-CG method terminates in one of the fall back cases).

When α is the Cauchy stepsize $\alpha = \frac{\delta}{\theta}$, this expression simplifies to $-\frac{1}{2}\alpha\delta$, so a successfull CG step requires 3 floating point operations to update the cost functional value.

Since the Steihaug-Toint CG is initialized at 0, we know that the initial iterates function value coincides with c, so the initialization is just copying the constant (which is the function value of the function to be minimized in the trust region scheme and can be passed to the algorithm from the trust region routine). Accordingly, the algorithm can be expanded to read as

Algorithm 0.1 (Steihaug-Toint conjugate gradient method for the trust-region subproblem (6.17)).

Input: *model value* $q(0) = c \in \mathbb{R}$
Input: *negative model derivative* $-q'(0) = b \in \mathbb{R}^n$
Input: *symmetric matrix* H *(or matrix-vector products with* H*)*
Input: *s. p. d. matrix* M *(or matrix-vector products with* M^{-1}*)*
Input: *relative residual* ε_{rel}
Input: *trust-region radius* $\Delta > 0$
Output: *approximate solution of the trust-region subproblem* (6.17) *and quadratic model evaluation*

Set $\ell := 0$
Set $s^{(0)} := 0$ // zero initial guess
Set $\zeta^{(0)} := -b$ // evaluate the initial residual
Set $p^{(0)} := -M^{-1}\zeta^{(0)}$
Set $\delta^{(0)} := -(\zeta^{(0)})^\intercal p^{(0)}$ // $\delta^{(0)} = \|\zeta^{(0)}\|^2_{M^{-1}}$
Set $v^{(0)} := c = q(0)$
while $\delta^{(\ell)} \ge \varepsilon_{\text{rel}}^2 \delta^{(0)}$ **do** // check stopping criterion (6.19)
    Set $q^{(\ell)} := H p^{(\ell)}$
    Set $\theta^{(\ell)} := (q^{(\ell)})^\intercal p^{(\ell)}$
    if $\theta^{(\ell)} > 0$ **then**
        Set $\alpha^{(\ell)} := \delta^{(\ell)} / \theta^{(\ell)}$
        Set $s^{(\ell+1)} := s^{(\ell)} + \alpha^{(\ell)} p^{(\ell)}$
        if $\|s^{(\ell+1)}\|_M > \Delta$ **then** // iterate would leave the trust region
            Determine α^* as the positive solution of $\|s^{(\ell)} + \alpha\, p^{(\ell)}\|_M = \Delta$
            Set $s^{(\ell+1)} := s^{(\ell)} + \alpha^* p^{(\ell)}$ // go to the boundary of the trust region
            Set $v^{(\ell+1)} := v^{(\ell)} + \alpha^*(\frac{1}{2}\alpha^*\theta^{(\ell)} - \delta^{(\ell)})$
            Set $\ell := \ell + 1$
            Abort the **while** loop
        else

Set $\zeta^{(\ell+1)} := \zeta^{(\ell)} + \alpha^{(\ell)} q^{(\ell)}$
Set $p^{(\ell+1)} := -M^{-1}\zeta^{(\ell+1)}$
Set $\delta^{(\ell+1)} := -(\zeta^{(\ell+1)})^\intercal p^{(\ell+1)}$ *// $\delta^{(\ell+1)} = \|\zeta^{(\ell+1)}\|^2_{M^{-1}}$*
Set $\beta^{(\ell+1)} := \delta^{(\ell+1)} / \delta^{(\ell)}$
Set $p^{(\ell+1)} := p^{(\ell+1)} + \beta^{(\ell+1)}\, p^{(\ell)}$
Set $v^{(\ell+1)} := v^{(\ell)} - \frac{1}{2}\alpha^{(\ell)}\delta^{(\ell)}$
Set $\ell := \ell + 1$
end if
else
Determine α^* *as the positive solution of* $\|s^{(\ell)} + \alpha\, p^{(\ell)}\|_M = \Delta$
Set $s^{(\ell+1)} := s^{(\ell)} + \alpha^*\, p^{(\ell)}$ *// go to the boundary of the trust region*
Set $v^{(\ell+1)} := v^{(\ell)} + \alpha^*(\frac{1}{2}\alpha^*\theta^{(\ell)} - \delta^{(\ell)})$
Set $\ell := \ell + 1$
Abort the ***while*** *loop*
end if
end while
return $s^{(\ell)}, v^{(\ell)}$

(3 Points)

Homework Problem 7.3 (Spektrum Shift for Symmetric Matrices) 3 Points

Let $H \in \mathbb{R}^{n\times n}$ be a symmetric matrix and $M \in \mathbb{R}^{n\times n}$ be s. p. d. Discuss for which values of $\mu \in \mathbb{R}$ the matrix $H + \mu M$ is positive definite, -semidefinite or indefinite, respectively.

Solution.

The symmetric matrix $H \in \mathbb{R}^{n\times n}$ has a generalized spectral decomposition with respect to M as per Equations (2.10) and (2.11) of the lecture notes, i. e. there are an M-orthogonal matrix $V \in \mathbb{R}^{n\times n}$ and a diagonal matrix $\Lambda \in \mathbb{R}^{n\times n}$ such that

$$H\,V = M\,V\Lambda \quad \text{i. e.,} \quad H = M\,V\Lambda V^\intercal M.$$

The diagonal of Λ holds the generalized eigenvalues $\lambda_1 \le \cdots \le \lambda_n$ of H w.r.t. M. The shift of H by μM shifts the spektrum of H w.r.t. M by μ. This is clear from looking at the generalized eigenvalue problem, but we can also show that of course the spectral decomposition is simply shifted, as

$$H + \mu M = M\,V\Lambda V^\intercal M + \mu M M^{-1} M = M\,V\Lambda V^\intercal M + \mu \mathrm{Id} M V V^\intercal M = M\,V(\Lambda + \mu\mathrm{Id})V^\intercal M$$

where the diagonal matrix $(\Lambda + \mu \mathrm{Id})$ now contains the generalized eigenvalues $\lambda_1 + \mu \leq \cdots \leq \lambda_n + \mu$. I. e., for $\mu \in (-\infty, -\lambda_n)$ and $(-\lambda_1, \infty)$, the modified matrix $H + \mu M$ is negative/positive definite and the border cases of semidefiniteness occur exactly for $\mu \in \{-\lambda_n, -\lambda_1\}$. In the remaining case that $\mu \in (-\lambda_n, -\lambda_1)$ (if there are at least two destinct generalized eigenvalues), there are negative and positive generalized eigenvalues, meaning that the matrix is indefinite, as $v_i^\intercal H v_i = (\lambda_i + \mu) v_i^\intercal M v < 0$ and $v_j^\intercal H v_j = (\lambda_i + \mu) v_j^\intercal M v_j > 0$ for some i, j such that $-\lambda_j < \mu < -\lambda_i$.

(3 Points)

Homework Problem 7.4 (Implementation of a Trust-Region-Method with Steihaug-CG) 6 Points

Implement a Newton-trust-region-method according to Algorithm 6.1 with Steihaug-Toint-CG (Algorithm 6.14). Keep a record of the trust region radius and the reduction ratio for visualization later. Apply your implementation to Rosenbrock's and/or Himmelblau's and discuss the results.

Solution.

For the implementation, see driver_ex_028_compare_trust_region_newton.py.

The trust region Newton method displays the typical second order method's convergence behavior.

Similarly to the accepted step sizes, the trust region radii settle in after a phase of being improved consecutively with short "bursts" of having to be pulled back after over enthusiastic enlargement of the trust region.

Note that the number of iterations needed until the algorithms terminate are of course largely parameter dependent, so the fact that the trust region method required about twice the iterations that the truncate Newton CG method required should not lead to the conclusion that the trust region version is slower. Epecially, since it counts unsuccesfull iterations (which require one function evaluation per iteration) while rejected step lengths in the armijo backtracking of the truncated Newton CG are not counted (which also require one function evaluation per iteration).

(6 Points)

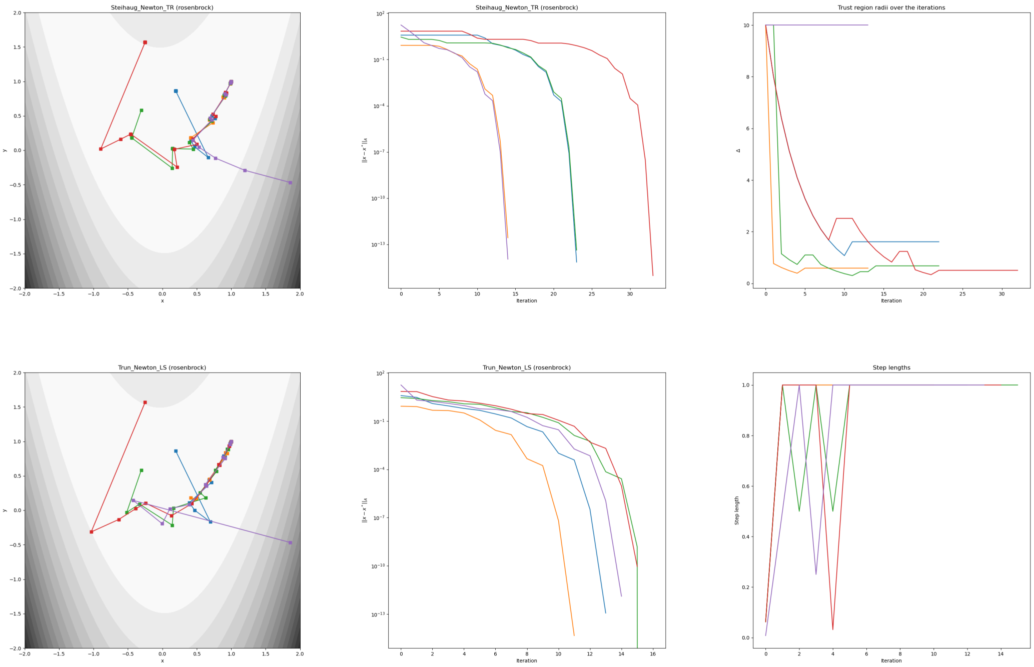

Figure 0.3: Convergence behavior of Steihaug-Newton trust-region method (top) and Truncated Newton CG (bottom) for Rosenbrock's function.

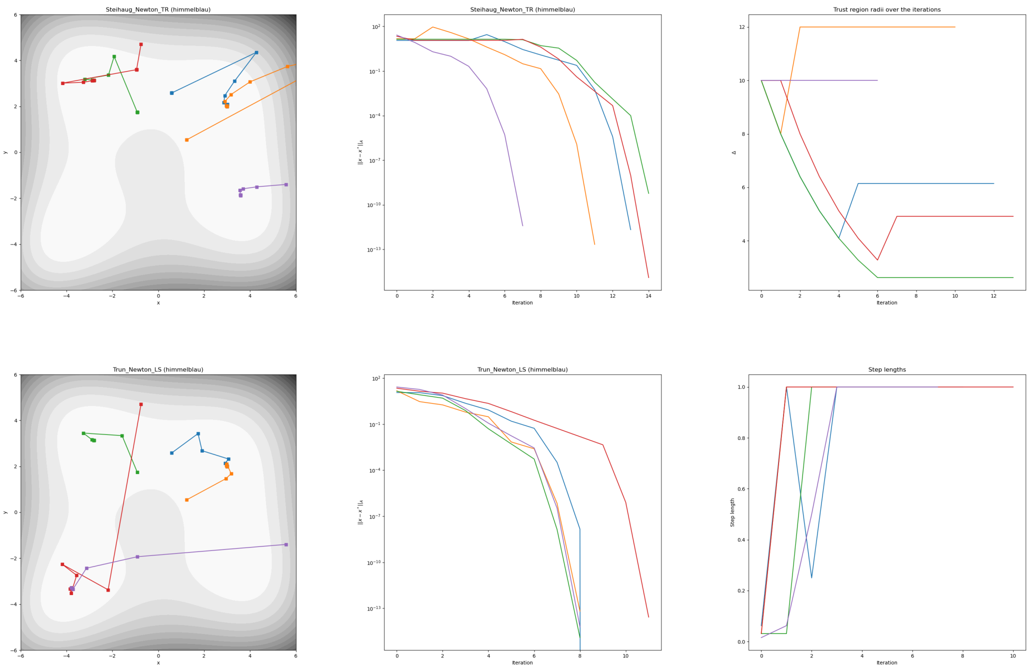

Figure 0.4: Convergence behavior of Steihaug-Newton trust-region method (top) and Truncated Newton CG (bottom) for Himmelblau's function.

Please submit your solutions as a single pdf and an archive of programs via moodle.