R. Herzog, G. Müller, E. Herberg, M. Hashemi
Heidelberg University

Exercise 2 - Solution

Date issued: 24th April 2023
Date due: 3rd May 2023

Homework Problem 2.1 (Solvability of quadratic polynomial minimization) 5 Points

Prove Lemma 4.1 of the lecture notes, i. e., the following statements for the optimization problem

$$\text{Minimize} \quad \phi(x) := \frac{1}{2} x^\mathsf{T} A\, x - b^\mathsf{T} x + c \quad \text{where } x \in \mathbb{R}^n \tag{4.1}$$

with symmetric $A \in \mathbb{R}^{n \times n}$, $b \in \mathbb{R}^n$ and $c \in \mathbb{R}$:

(i) If A is positive semidefinite, then the objective in (4.1) is convex. In this case, the following are equivalent:

   (a) The problem (4.1) possess at least one (global) minimizer.

   (b) The objective ϕ is bounded below.

   (c) $A\,x = b$ is solvable.

   The global minimizers of (4.1) are precisely the solutions of the linear system $A\,x = b$.

(ii) In case A is not positive semidefinite, the objective ϕ is not bounded below, thus problem (4.1) is unbounded.

Solution.

(i) Since ϕ is $C^\infty(\mathbb{R}^n, \mathbb{R})$, we can resort to the characterization of convexity via the second derivative, which is $\phi'' \equiv A$ and therefore positive semidefinite by assumption, yielding convexity. This implies that all local minimizers are global ones.

As for the equivalences: Statement (c) is the first order optimality condition at x for the problem (4.1), which, due to the convexity of the problem, is equivalent to x being a minimizer – i. e. "Statement (c) $\Leftrightarrow$ statement (a)". (1 Point)

"Statement (a) $\Rightarrow$ statement (b)" is trivial because the infimal value of the function is the function value of the minimizer and therefore real valued. (0.5 Points)

For "Statement (b) $\Rightarrow$ statement (a)", assume boundedness of ϕ from below. Then $b \in \ker(A)^\perp$ (with orthogonality respective to the euclidean scalar product), because otherwise there were an $x \in \ker(A)$ with $b^\intercal x > 0$ and $\phi(\lambda x) \xrightarrow{\lambda\to\infty} -\infty$. Now let's also assume that $A \neq 0$, otherwise every point is a minimizer anyway. Now take an infimizing sequence $\left(x^{(k)}\right)$, i. e.:

$$\lim_{k\to\infty} \phi(x^{(k)}) = \inf_{x\in\mathbb{R}^n} \phi(x) \in \mathbb{R}.$$

The elements of the sequence can be split up into $x^{(k)} = x^{(k)}_{\ker} + x^{(k)}_\perp$ for respective elements in $\ker(A)$ and $\ker(A)^\perp$. Since $\phi(x^{(k)}) = \phi(x^{(k)}_\perp)$, the sequence $\left(x^{(k)}_\perp\right)$ is an infimizing sequence as well. Since

$$\phi(x^{(k)}_\perp) = \frac{1}{2} x^{(k)^\intercal}_\perp A x^{(k)}_\perp - b^\intercal x^{(k)}_\perp + c \geq \lambda_{\min} \|x^{(k)}_\perp\|^2 - \|b\| \|x^{(k)}_\perp\| + c \xrightarrow{\|x^{(k)}_\perp\|\to\infty} \infty$$

for $\lambda_{\min}$ being the smallest nonzero eigenvalue of A, $x^{(k)}_\perp$ needs to be bounded. Accordingly, it has a convergent subsequence whose limit point is a minimizer. (2 Points)

Since $Ax = b$ is the first order optimality condition, which is necessary and sufficient in the convex case, the solutions to the linear system are precisely the (global) minimizers.

(ii) When A is not positive semidefinite, it has a negative eigenvalue $\lambda < 0$ with corresponding eigenvector $x_\lambda \in \mathbb{R}^n$ and

$$\phi(tx_\lambda) = \frac{1}{2} x_\lambda^\intercal A x_\lambda t^2 - b^\intercal x_\lambda t + c = \underbrace{\lambda \frac{1}{2} \|x_\lambda\|^2}_{<0} t^2 - b^\intercal x_\lambda t + c \xrightarrow{t\to\pm\infty} -\infty.$$

(1.5 Points)

Homework Problem 2.2 (M-steepest descent directions coincide with descent directions) 10 Points

(i) Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be differentiable at $x \in \mathbb{R}^n$ with $f'(x) \neq 0$. Show that the set of directions of steepest descent of f at x w.r.t. all inner product conincides with the set of descent directions, i. e., that

$$\{-M^{-1}\nabla f(x) \mid M \in \mathbb{R}^{n\times n} \text{ s.p.d.}\} = \{d \in \mathbb{R}^n \mid f'(x)d < 0\}.$$

Hint: For any $g, d \in \mathbb{R}^n$ such that $g^\intercal d > 0$ and starting with any s.p.d. matrix M, the low rank modifications

$$\tilde{M} \coloneqq \left(\mathrm{Id} - \frac{gd^\intercal}{g^\intercal d}\right) M \left(\mathrm{Id} - \frac{dg^\intercal}{g^\intercal d}\right) + \frac{gg^\intercal}{g^\intercal d} \tag{DFP}$$

$$\tilde{M} \coloneqq M - \frac{Mdd^\intercal M}{d^\intercal M d} + \frac{gg^\intercal}{g^\intercal d} \tag{BFGS}$$

yield s.p.d. matrices $\tilde{M}$ with $\tilde{M}d = g$.

(ii) Implement a method `compute_gradient(derivative, preconditioner)` that computes the M-gradient corresponding to a derivative $f'(x)$ and a preconditioner M and use it to visualize the result from task (i).

Solution.

(i) For the inclusion $\{-M^{-1}\nabla f(x) \mid M \in \mathbb{R}^{n\times n} \text{ s.p.d.}\} \subseteq \{d \in \mathbb{R}^n \mid f'(x)d < 0\}$ notice that, for any s.p.d. $M \in \mathbb{R}^{n\times n}$, we have that

$$f'(x)\left(M^{-1}\nabla f(x)\right) = \nabla f(x)^\intercal M^{-1} M M^{-1} \nabla f(x) = \left(M^{-1}\nabla f(x)\right)^\intercal M M^{-1}\nabla f(x) = \|M^{-1}\nabla f(x)\|_M^2 > 0.$$

(1 Point)

For the inclusion $\{-M^{-1}\nabla f(x) \mid M \in \mathbb{R}^{n\times n} \text{ s.p.d.}\} \supseteq \{d \in \mathbb{R}^n \mid f'(x)d < 0\}$ let d with $f'(x)d < 0$ be given. We need to find an s.p.d. $M \in \mathbb{R}^{n\times n}$ such that $Md = -\nabla f(x) \eqqcolon g$. Note that this is solving a linear system of equations *for the matrix* under the additional requirement, that the matrix be s.p.d. That is part of the job that quasi-Newton update procedures take care of (they solve these problems with the additional constraint that these updates are closest to M in some norm), so we can employ, e. g., BFGS- or DFP-style modifications of any initial s.p.d. matrix. Both obviously generate symmetric matrices. Additionally, by assumption, we have that $g^\intercal d = -f'(x)d > 0$.

For the DFP update, we obtain positive semidefiniteness of the matrix by choosing $v \in \mathbb{R}^n$ and noting that

$$v^\top \tilde{M} v = v^\top \left(\mathrm{Id} - \frac{g d^\top}{g^\top d}\right) M \left(\mathrm{Id} - \frac{d g^\top}{g^\top d}\right) v + \frac{v^\top g\, g^\top v}{g^\top d} = \left(v^\top - \frac{v^\top g d^\top}{g^\top d}\right) M \left(v - \frac{d g^\top v}{g^\top d}\right) + \frac{v^\top g\, g^\top v}{g^\top d} \geq 0$$

because both summands are greater or equal to zero seperately. For any v where the inequality holds as an equality, necessarily the first summand has to be zero itself, i. e.,

$$v = \frac{d g^\top v}{g^\top d}$$

which means that v is a multiple of d. Since the second term is zero as well, which means that $g^\top v = 0$, and since $g^\top d \neq 0$, we know that v is 0, showing positive definiteness. (1.5 Points)
Additionally,

$$\tilde{M} d = \left(\mathrm{Id} - \frac{g d^\top}{g^\top d}\right) M \underbrace{\left(\mathrm{Id} - \frac{d g^\top}{g^\top d}\right) d}_{=0} + \underbrace{\frac{g\, g^\top d}{g^\top d}}_{=g} = g$$

as expected. I. e., we can simply choose the identy matrix as M and compute the DFP update. (1 Point)

Alternatively, one can use the BFGS update but proving that this is positive definite is best done by knowing that its inverse has reciprocal structure to the DFP update (d and g switch roles) and proceeding as above.

Showing that $\tilde{M} d = g$ for the BFGS-Update is easy however, as

$$\tilde{M} d = \underbrace{M d - \frac{M d d^\top M d}{d^\top M d}}_{=0} + \underbrace{\frac{g g^\top d}{g^\top d}}_{=g} = g.$$

(ii) See driver_ex_004_preconditioned_gradients_visualization.py. (6.5 Points)

Homework Problem 2.3 (Implications of Termination Criteria) 4 Points

Prove Lemma 4.11 of the lecture notes, i. e., that when implementing an M-gradient descent scheme for solving s.p.d. quadratic problems with Matrix A, then

$$\|r^{(k)}\|_{M^{-1}} \le \varepsilon_{\text{rel}}\,\|r^{(0)}\|_{M^{-1}} \quad\Rightarrow\quad \begin{cases} \|x^{(k)} - x^*\|_A \le \sqrt{\kappa}\,\varepsilon_{\text{rel}}\,\|x^{(0)} - x^*\|_A \\ \|x^{(k)} - x^*\|_M \le \kappa\,\varepsilon_{\text{rel}}\,\|x^{(0)} - x^*\|_M \end{cases},$$

$$\|r^{(k)}\|_{M^{-1}} \le \varepsilon_{\text{abs}} \quad\Rightarrow\quad \begin{cases} \|x^{(k)} - x^*\|_A \le (1/\sqrt{\alpha})\,\varepsilon_{\text{abs}} \\ \|x^{(k)} - x^*\|_M \le (1/\alpha)\,\varepsilon_{\text{abs}} \end{cases},$$

$$\|r^{(k)}\|_{M^{-1}} \le \varepsilon_{\text{rel}}\,\|r^{(0)}\|_{M^{-1}} + \varepsilon_{\text{abs}} \quad\Rightarrow\quad \begin{cases} \|x^{(k)} - x^*\|_A \le \sqrt{\kappa}\,\varepsilon_{\text{rel}}\,\|x^{(0)} - x^*\|_A + (1/\sqrt{\alpha})\,\varepsilon_{\text{abs}} \\ \|x^{(k)} - x^*\|_M \le \kappa\,\varepsilon_{\text{rel}}\,\|x^{(0)} - x^*\|_M + (1/\alpha)\,\varepsilon_{\text{abs}} \end{cases},$$

$$\|r^{(k)}\|_{M^{-1}} \le \max\bigl\{\varepsilon_{\text{rel}}\,\|r^{(0)}\|_{M^{-1}},\ \varepsilon_{\text{abs}}\bigr\} \quad\Rightarrow\quad \begin{cases} \|x^{(k)} - x^*\|_A \le \max\bigl\{\sqrt{\kappa}\,\varepsilon_{\text{rel}}\,\|x^{(0)} - x^*\|_A,\ (1/\sqrt{\alpha})\,\varepsilon_{\text{abs}}\bigr\} \\ \|x^{(k)} - x^*\|_M \le \max\bigl\{\kappa\,\varepsilon_{\text{rel}}\,\|x^{(0)} - x^*\|_M,\ (1/\alpha)\,\varepsilon_{\text{abs}}\bigr\} \end{cases},$$

where $\alpha := \lambda_{\min}(A;M)$ and $\beta := \lambda_{\max}(A;M)$ are the extremal generalized eigenvalues of A w.r.t. M, and $\kappa := \frac{\beta}{\alpha}$ is the generalized condition number.

Solution.

The relation

$$A\,(x^{(k)} - x^*) = A\,x^{(k)} - b = r^{(k)}$$

for the error and the residual implies that

$$\|r^{(k)}\|_{M^{-1}}^2 = r^{(k)\mathsf{T}} M^{-1} r^{(k)} = (x^{(k)} - x^*)^\mathsf{T} A\,M^{-1} A\,(x^{(k)} - x^*) = \|x^{(k)} - x^*\|_{A\,M^{-1}A}^2.$$

The left hand side conditions can therefore be equivalently stated replacing the residual norm. (1 Point)

Additionally, the generalized Rayleigh quotient estimates in Equations (2.10b) and (2.8) state that

$$\alpha \le \frac{x^\mathsf{T} A\,M^{-1} A\,x}{x^\mathsf{T} A\,x} \le \beta \quad \text{for all } x \neq 0,$$
$$\alpha \le \frac{x^\mathsf{T} A\,x}{x^\mathsf{T} M\,x} \le \beta \quad \text{for all } x \neq 0$$

which means that

$$\begin{aligned} \sqrt{\alpha}\|x\|_A &\le \|x\|_{A\,M^{-1}A} \le \sqrt{\beta}\|x\|_A, \\ \sqrt{\alpha}\|x\|_M &\le \|x\|_A \qquad\quad\, \le \sqrt{\beta}\|x\|_M, \end{aligned},$$

and therefore

$$\begin{aligned} \sqrt{\alpha}\|x\|_A &\le \|x\|_{A\,M^{-1}A} \le \sqrt{\beta}\|x\|_A, \\ \alpha\|x\|_M &\le \|x\|_{A\,M^{-1}A} \le \beta\|x\|_M, \end{aligned}$$

(1 Point)

We can apply these estimates to obtain that

$$\begin{aligned}
\|r^{(k)}\|_{M^{-1}} \le \varepsilon_{\text{rel}} \|r^{(0)}\|_{M^{-1}} &\Rightarrow \|x^{(k)} - x^*\|_{A M^{-1} A} \le \varepsilon_{\text{rel}} \|x^{(0)} - x^*\|_{A M^{-1} A} \\
&\Rightarrow \begin{cases} \sqrt{\alpha}\|x^{(k)} - x^*\|_A \le \sqrt{\beta}\, \varepsilon_{\text{rel}} \|x^{(0)} - x^*\|_A \\ \alpha\|x^{(k)} - x^*\|_M \le \beta\, \varepsilon_{\text{rel}} \|x^{(0)} - x^*\|_M \end{cases} \\
&\Rightarrow \begin{cases} \|x^{(k)} - x^*\|_A \le \sqrt{\kappa}\, \varepsilon_{\text{rel}} \|x^{(0)} - x^*\|_A \\ \|x^{(k)} - x^*\|_M \le \kappa\, \varepsilon_{\text{rel}} \|x^{(0)} - x^*\|_M \end{cases},
\end{aligned}$$

which is the first implication.

Analogously, we obtain the second implication because

$$\begin{aligned}
\|r^{(k)}\|_{M^{-1}} \le \varepsilon_{\text{abs}} &\Rightarrow \|x^{(k)} - x^*\|_{A M^{-1} A} \le \varepsilon_{\text{abs}} \\
&\Rightarrow \begin{cases} \sqrt{\alpha}\|x^{(k)} - x^*\|_A \le \varepsilon_{\text{abs}} \\ \alpha\|x^{(k)} - x^*\|_M \le \varepsilon_{\text{abs}} \end{cases} \\
&\Rightarrow \begin{cases} \|x^{(k)} - x^*\|_A \le (1/\sqrt{\alpha})\, \varepsilon_{\text{abs}} \\ \|x^{(k)} - x^*\|_M \le (1/\alpha)\, \varepsilon_{\text{abs}} \end{cases}.
\end{aligned}$$

For the remaining implications, simply combine the steps of the first and second implications. (2 Points)

Homework Problem 2.4 (M-Gradient Method for Solving s.p.d. Linear Systems) 8 Points

Implement the M-gradient descent method as outlined in Algorithm 4.6 of the lecture notes. Additionally, include the option of supplying different methods for choosing the step sizes. Visualize the effects of different choices of the preconditioner, step size strategies and initial values.

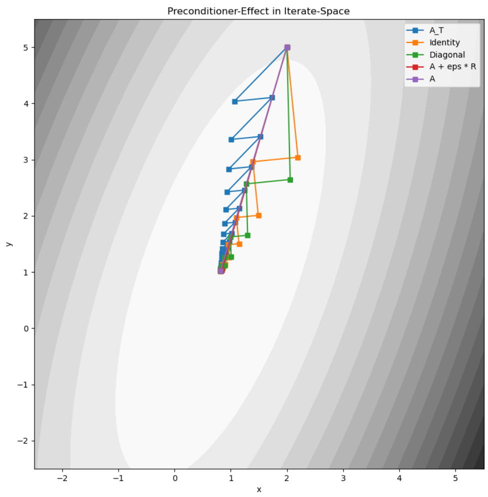
Solution.

For the implementation, see driver_ex_008_gradient_descent_quadratic_visualization.py.

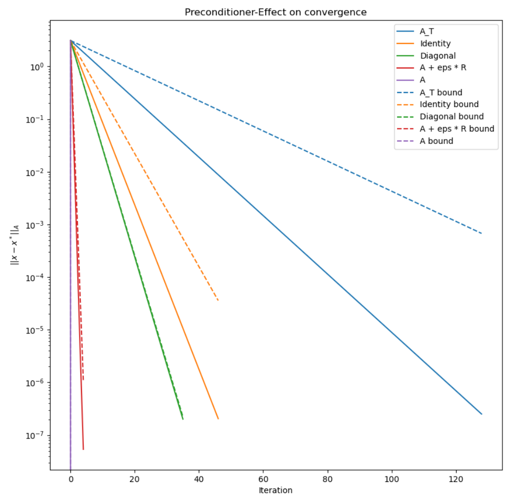
For the preconditioners, we fix the cauchy step size strategy and consider

$$M \in \{A_{\mathsf{T}}, \mathrm{Id}, \mathrm{diag}(\mathrm{diag}(A)), A + R, A\}$$

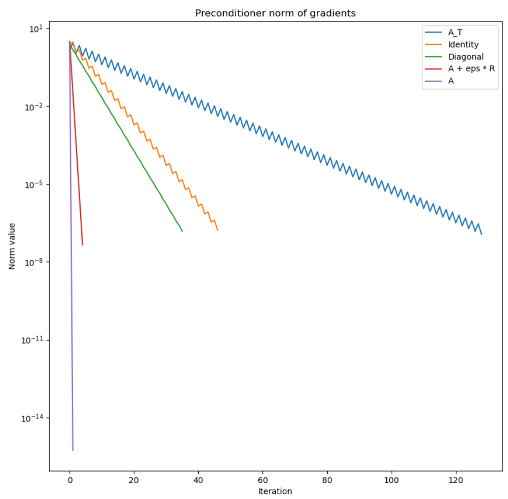
where A_{T} is the transpose of A across the antidiagonal and R is a pseudo randomly generated s.p.d. matrix. As shown in Figure 0.1, the performance is greatly influenced by the preconditioners and is



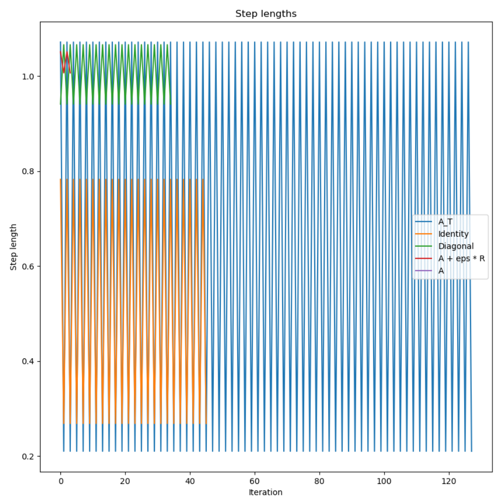
(a) Iterates for various preconditioners.



(b) Error $\|x^{(k)} - x^*\|_A$. Dashed lines indicate the linear convergence bound.

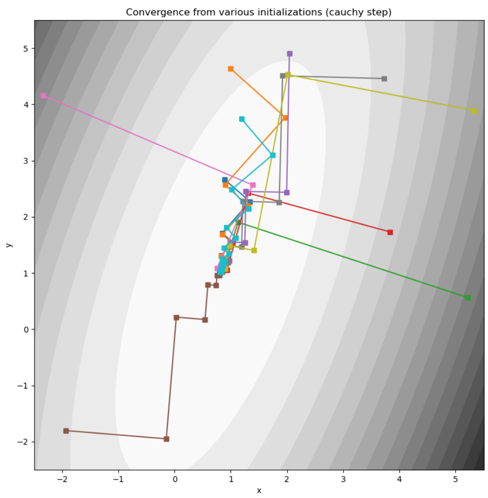


(c) Norm of the gradients $\|\nabla_M f(x^{(k)})\|_M = \|r^{(k)}\|_{M^{-1}}$.

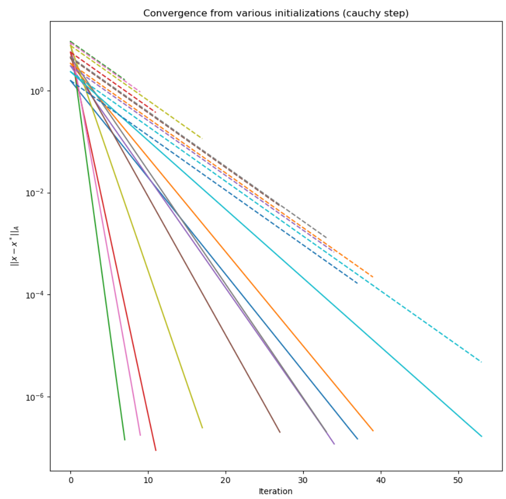


(d) Third subfigure.

Figure 0.1: Visualization of Preconditioner Influence.



(a) Iterates for various preconditioners.



(b) Error $\|x^{(k)} - x^*\|_A$. Dashed lines indicate the linear convergence bound.

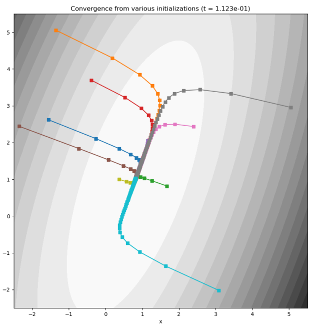
Figure 0.2: Visualization of the Initial Value Influence.

improved by those that capture the essence of A reasonably, such as A itself, a small permutation $A + R$ of A and its diagonal. The antitranspose captures the essence of A even worse than the identity does, leading to more zig-zagging and generally slower convergence.

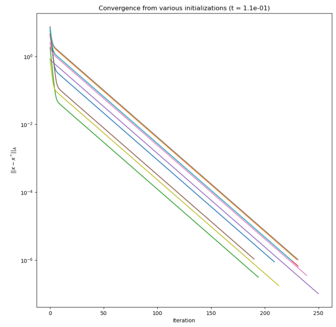
For the initial values, the results match those of the lecture notes, where the choice of the initial value highly influences the convergence speed while the upper bound remains unchanged by the choices, see Figure 0.2.

When considering various fixed step size strategies for steps in $(0, 2/\beta)$, the results match those of the lecture notes, see Figure 0.3. While small step sizes lead to a gradient-flow like sequence of iterates, choosing the step size too large will result in eradic behavior and more and more initial values tend to yield slow convergence. Choosing the step length only slightly larger than $2/\beta$ will immediately yield non-convergence for some initial values. (8 Points)

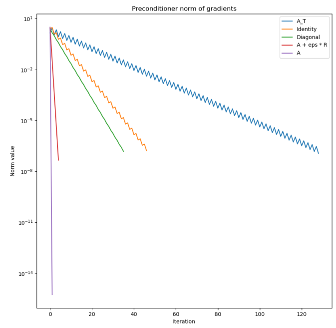
Please submit your solutions as a single pdf and an archive of programs via moodle.



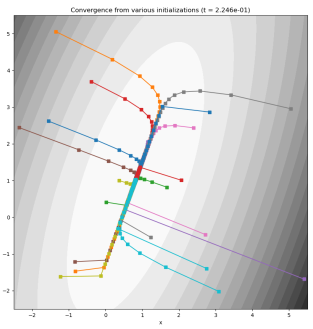
(a) Iterates for various preconditioners.



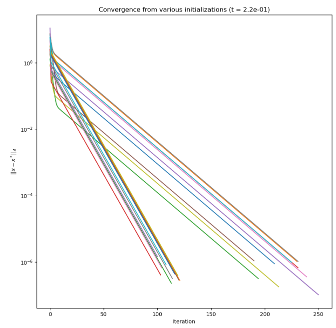
(b) Error $\|x^{(k)} - x^*\|_A$.



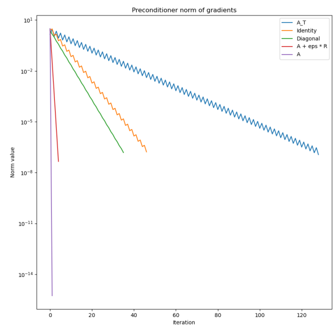
(c) Norm of the gradients $\|\nabla_M f(x^{(k)})\|_M = \|r^{(k)}\|_{M^{-1}}$.



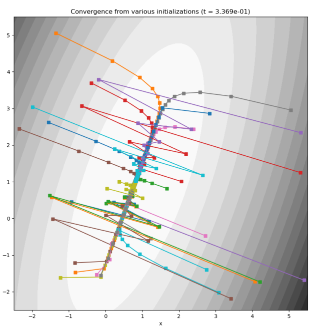
(d) Iterates for various preconditioners.



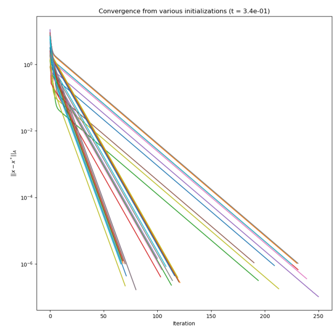
(e) Error $\|x^{(k)} - x^*\|_A$.



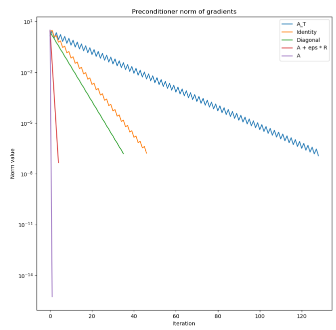
(f) Norm of the gradients $\|\nabla_M f(x^{(k)})\|_M = \|r^{(k)}\|_{M^{-1}}$.



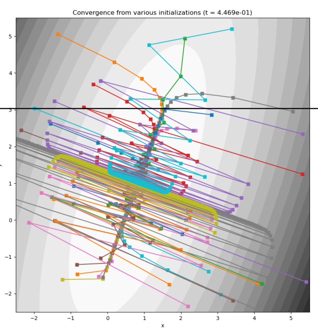
(g) Iterates for various preconditioners.



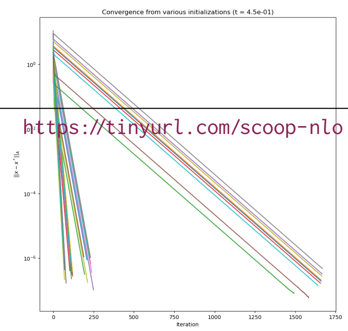
(h) Error $\|x^{(k)} - x^*\|_A$.



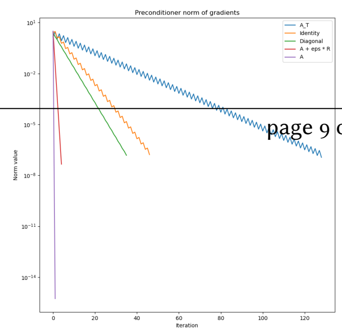
(i) Norm of the gradients $\|\nabla_M f(x^{(k)})\|_M = \|r^{(k)}\|_{M^{-1}}$.



(j) Iterates for various preconditioners.



(k) Error $\|x^{(k)} - x^*\|_A$.



(l) Norm of the gradients $\|\nabla_M f(x^{(k)})\|_M = \|r^{(k)}\|_{M^{-1}}$.

Figure 0.3: Visualization of the influence of fixed step lengths $2/\beta\{\frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1-\varepsilon\}$, top to bottom.