Numerical Optimization

Unconstrained Optimization

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NPTEL Course on Numerical Optimization

Consider the problem to minimize

$$\min \ f(\boldsymbol{x}) \triangleq \frac{1}{2}\boldsymbol{x}^T \boldsymbol{H}\boldsymbol{x} - \boldsymbol{c}^T \boldsymbol{x}$$

where $\boldsymbol{H}$ is a symmetric positive definite matrix.

- *Condition number* of the Hessian matrix controls the convergence rate of steepest descent method.
- Faster convergence if the Hessian matrix is $\boldsymbol{I}$
- Let $\boldsymbol{H} = \boldsymbol{L}\boldsymbol{L}^T$ be the Cholesky decomposition of $\boldsymbol{H}$
- Define $\boldsymbol{y} = \boldsymbol{L}^T\boldsymbol{x}$. Therefore, the function $f(\boldsymbol{x})$ is transformed to the function $h(\boldsymbol{y})$.

$$h(\boldsymbol{y}) \triangleq f(\boldsymbol{L}^{-T}\boldsymbol{y})$$

$$
\begin{aligned}
h(\boldsymbol{y}) &= f(\boldsymbol{L}^{-T}\boldsymbol{y}) \\
&= \frac{1}{2}\boldsymbol{y}^T\boldsymbol{L}^{-1}\boldsymbol{H}\boldsymbol{L}^{-T}\boldsymbol{y} - \boldsymbol{c}^T\boldsymbol{L}^{-T}\boldsymbol{y} \\
&= \frac{1}{2}\boldsymbol{y}^T\boldsymbol{L}^{-1}\boldsymbol{L}\boldsymbol{L}^T\boldsymbol{L}^{-T}\boldsymbol{y} - \boldsymbol{c}^T\boldsymbol{L}^{-T}\boldsymbol{y} \\
&= \frac{1}{2}\boldsymbol{y}^T\boldsymbol{y} - \boldsymbol{c}^T\boldsymbol{L}^{-T}\boldsymbol{y}
\end{aligned}
$$

- The Hessian matrix of $h(\boldsymbol{y})$ is $\boldsymbol{I}$
- Let us apply steepest descent method in $\boldsymbol{y}$-space

$$
\begin{aligned}
\boldsymbol{y}^{k+1} &= \boldsymbol{y}^k - \nabla h(\boldsymbol{y}^k) \\
&= \boldsymbol{y}^k - \boldsymbol{L}^{-1}\nabla f(\boldsymbol{L}^{-T}\boldsymbol{y}^k) \\
\therefore \boldsymbol{L}^{-T}\boldsymbol{y}^{k+1} &= \boldsymbol{L}^{-T}\boldsymbol{y}^k - \boldsymbol{L}^{-T}\boldsymbol{L}^{-1}\nabla f(\boldsymbol{L}^{-T}\boldsymbol{y}^k) \\
\therefore \boldsymbol{x}^{k+1} &= \boldsymbol{x}^k - \boldsymbol{H}^{-1}\nabla f(\boldsymbol{x}^k)
\end{aligned}
$$

Newton Method

Consider the problem,

$$\min_{\boldsymbol{x}} \ f(\boldsymbol{x})$$

- Let $f \in \mathcal{C}^2$ and f be bounded below.
- Use second order information to find a descent direction
- At every iteration, use Taylor series to approximate f at $\boldsymbol{x}^k$ by a quadratic function and find the minimum of this quadratic function to get $\boldsymbol{x}^{k+1}$

$$\begin{aligned} f(\boldsymbol{x}) \approx f_q(\boldsymbol{x}) &= f(\boldsymbol{x}^k) + \boldsymbol{g}^{k^T}(\boldsymbol{x} - \boldsymbol{x}^k) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^k)^T \boldsymbol{H}^k (\boldsymbol{x} - \boldsymbol{x}^k) \\ \boldsymbol{x}^{k+1} &= \arg\min_{\boldsymbol{x}} \ f_q(\boldsymbol{x}) \end{aligned}$$

- $\nabla f_q(\boldsymbol{x}) = 0 \ \Rightarrow \ \boldsymbol{x}^{k+1} = \boldsymbol{x}^k - (\boldsymbol{H}^k)^{-1}\boldsymbol{g}^k$ (assuming $\boldsymbol{H}^k$ is invertible)

$x^{k+1} = x^k - (H^k)^{-1} g^k$ is of the form, $x^{k+1} = x^k + \alpha^k d^k$

- Classical Newton Method:
  - Newton Direction: $d_N^k = -(H^k)^{-1} g^k$
  - Step Length: $\alpha^k = 1$
- Is d_N^k a descent direction?
  $g^{k^T} d_N^k = -g^{k^T} (H^k)^{-1} g^k < 0$ if H^k is positive definite.

  d_N^k is a descent direction if H^k is positive definite
- Consider the problem to minimize, $f(x) = \frac{1}{2} x^T H x - c^T x$ where H is a symmetric positive definite matrix.
  $g(x) = 0 \ \Rightarrow \ x^* = H^{-1} c$ is a strict local minimum
  Let $x^0 \in \mathbb{R}^n$ be any point. $g(x^0) = Hx^0 - c, \ H(x^0) = H$.
  Using classical Newton method,
  $x^1 = x^0 - H^{-1}(Hx^0 - c) = H^{-1} c = x^*$.

  Using classical newton method, the minimum of a strictly convex quadratic function (with invertible Hessian matrix) is attained in one iteration from *any starting point*.

Classical Newton Algorithm

(1) Initialize $\boldsymbol{x}^0$ and ϵ, set $k := 0$.

(2) **while** $\|\boldsymbol{g}^k\| > \epsilon$

  (a) $\boldsymbol{d}^k = -(\boldsymbol{H}^K)^{-1}\boldsymbol{g}^k$

  (b) $\alpha^k = 1$

  (c) $\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \alpha^k\boldsymbol{d}^k$

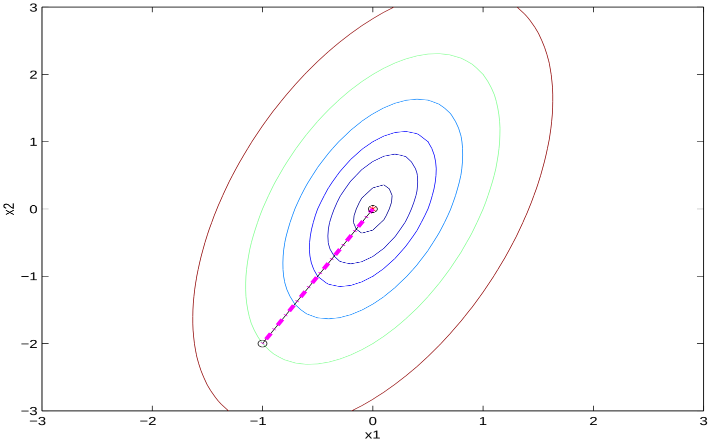
  (d) $k := k + 1$

endwhile

Output : $\boldsymbol{x}^* = \boldsymbol{x}^k$, a stationary point of $f(\boldsymbol{x})$.

Example:

$$\min \quad f(\boldsymbol{x}) \triangleq 4x_1^2 + x_2^2 - 2x_1x_2$$



Classical Newton algorithm applied to $f(\boldsymbol{x})$ converges to $\boldsymbol{x}^*$ in one iteration from any starting point

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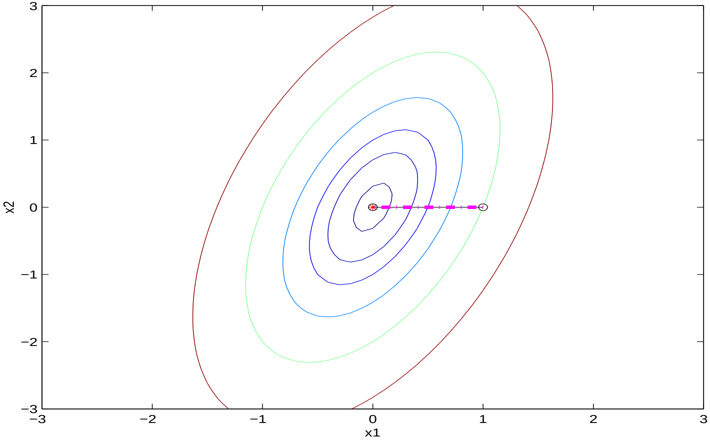
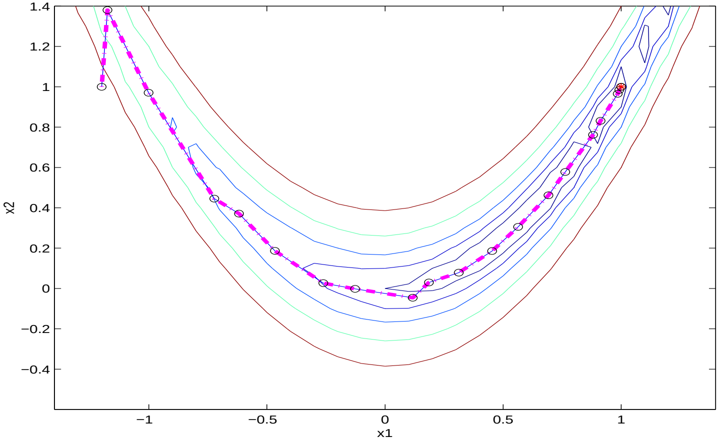


Classical Newton algorithm applied to $f(\boldsymbol{x})$ converges to $\boldsymbol{x}^*$ in one iteration from any starting point

Example (Rosenbrock function):

$$\min \quad f(\boldsymbol{x}) \stackrel{\Delta}{=} 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



Behaviour of classical Newton algorithm (with backtracking line search) applied to $f(\boldsymbol{x})$ using $\boldsymbol{x}^0 = (-1.2, 1)^T$

Example (Rosenbrock function):

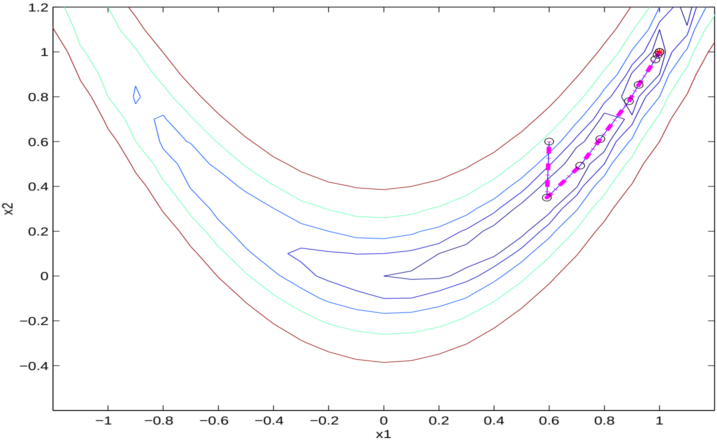
$$\min \quad f(\boldsymbol{x}) \triangleq 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

k	x_1^k	x_2^k	$f(\boldsymbol{x}^k)$	$\|\boldsymbol{g}^k\|$	$\|\boldsymbol{x}^k - \boldsymbol{x}^*\|$
0	-1.2	1	24.2	232.86	2.2
1	-1.17	1.38	4.73	4.64	2.21
2	-1.00	0.97	4.01	17.54	2.00
3	-0.72	0.45	3.57	30.06	1.81
4	-0.62	0.37	2.63	6.34	1.74
5	-0.47	0.19	2.24	10.64	1.68
10	0.31	0.08	0.51	4.00	1.15
15	0.88	0.76	0.03	5.37	0.27
20	0.99	0.99	7.38×10^{-13}	1.3×10^{-6}	1.9×10^{-6}

Table: Classical Newton algorithm (with backtracking line search) applied to Rosenbrock function, using $\boldsymbol{x}^0 = (-1.2, 1.0)^T$, $\hat{\alpha} = 1$, $\rho = .3$ and $c_1 = 1.0 \times 10^{-4}$.

Example (Rosenbrock function):

$$\min \quad f(\boldsymbol{x}) \stackrel{\Delta}{=} 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



Behaviour of classical Newton algorithm (with backtracking line search) applied to $f(\boldsymbol{x})$ using $\boldsymbol{x}^0 = (0.6, 0.6)^T$

Example (Rosenbrock function):

$$\min \; f(\boldsymbol{x}) \triangleq 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

k	x_1^k	x_2^k	$f(\boldsymbol{x}^k)$	$\|\boldsymbol{g}^k\|$	$\|\boldsymbol{x}^k - \boldsymbol{x}^*\|$
0	0.6	0.6	5.92	75.5947	0.57
1	0.59	0.35	0.17	0.80	0.77
2	0.71	0.49	0.10	4.64	0.58
3	0.79	0.61	0.05	1.65	0.44
4	0.89	0.78	0.02	4.18	0.25
5	0.92	0.85	0.01	0.40	0.17
9	0.99	0.99	5.76×10^{-13}	2.77×10^{-6}	1.69×10^{-6}

Table: Classical Newton algorithm (with backtracking line search) applied to Rosenbrock function, using $\boldsymbol{x}^0 = (0.6, 0.6)^T, \hat{\alpha} = 1, \rho = .3$ and $c_1 = 1.0 \times 10^{-4}$.

Classical Newton Algorithm

(1) Initialize $\boldsymbol{x}^0$ and ϵ, set $k := 0$.

(2) **while** $\|\boldsymbol{g}^k\| > \epsilon$

  (a) $\boldsymbol{d}^k = -(\boldsymbol{H}^K)^{-1}\boldsymbol{g}^k$

  (b) $\alpha^k = 1$

  (c) $\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \alpha^k \boldsymbol{d}^k$

  (d) $k := k + 1$

endwhile

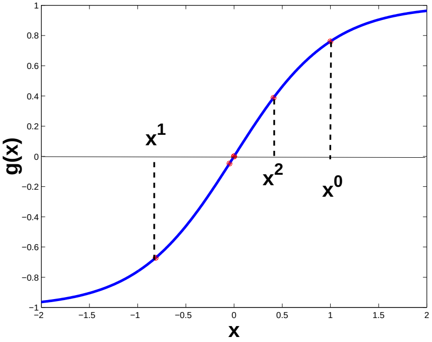
Output : $\boldsymbol{x}^* = \boldsymbol{x}^k$, a stationary point of $f(\boldsymbol{x})$.

- Requires $O(n^3)$ computational effort for every iteration (Step 2(a))
- *No guarantee* that $\boldsymbol{d}^k$ is a descent direction
- *No guarantee* that $f(\boldsymbol{x}^{k+1}) < f(\boldsymbol{x}^k)$ (no line search)
- Sensitive to initial point (for non-quadratic functions)

Consider the problem,

$$\min_{x \in \mathbb{R}} \quad \log(e^x + e^{-x})$$

- $f(x) = \log(e^x + e^{-x})$
- $g(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$



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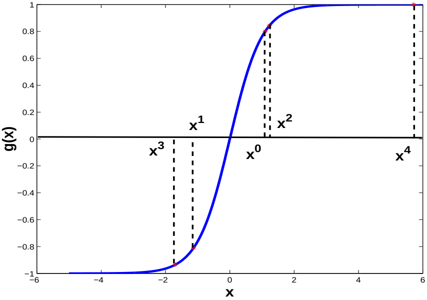

Classical Newton algorithm does not converge with this initialization of x^0

Definition

An iterative optimization algorithm is said to be locally convergent if for each solution $\boldsymbol{x}^*$, there exists $\delta > 0$ such that for any initial point $\boldsymbol{x}^0 \in B(\boldsymbol{x}^*, \delta)$, the algorithm produces a sequence $\{\boldsymbol{x}^k\}$ which converges to $\boldsymbol{x}^*$.

- Classical Newton algorithm is locally convergent

Let $f : \mathbb{R} \rightarrow \mathbb{R}$, $f \in \mathcal{C}^2$.
Consider the problem:

$$\min \quad f(x)$$

Let $x^* \in \mathbb{R}$ be such that $g(x^*) = 0$ and $g'(x^*) > 0$.
Assume that x^0 is *sufficiently* close to x^*.
Suppose we apply classical Newton algorithm to minimize $f(x)$.

At k-th iteration,

$$\begin{aligned} x^{k+1} &= x^k - \frac{g(x^k)}{g'(x^k)} \\ \therefore x^{k+1} - x^* &= x^k - x^* - \frac{g(x^k) - g(x^*)}{g'(x^k)} \\ &= -\frac{\left(g(x^k) - g(x^*) + g'(x^k)(x^* - x^k)\right)}{g'(x^k)} \end{aligned}$$

If we assume that $f \in \mathcal{C}^3$ (or $g \in \mathcal{C}^2$), then using truncated Taylor series,

$$g(x^*) = g(x^k) + g'(x^k)(x^* - x^k) + \frac{1}{2} g''(\bar{x}^k)(x^* - x^k)^2$$

where $\bar{x}^k \in LS(x^*, x^k)$.

Therefore,

$$x^{k+1} - x^* = \frac{1}{2} \frac{g''(\bar{x}^k)}{g'(x^k)} (x^k - x^*)^2$$

$$|x^{k+1} - x^*| = \frac{1}{2}\frac{|g''(\bar{x}^k)|}{|g'(x^k)|}|x^k - x^*|^2$$

Suppose there exist α_1 and α_2 such that

$$\begin{aligned} |g''(\bar{x}^k)| &< \alpha_1 \ \forall\, \bar{x}^k \in LS(x^*, x^k) \text{ and} \\ |g'(x^k)| &> \alpha_2 \ \text{ for } x^k \text{ sufficiently close to } x^*, \end{aligned}$$

then

$$|x^{k+1} - x^*| \leq \frac{\alpha_1}{2\alpha_2}|x^k - x^*|^2 \qquad \text{(order two convergence if} x^k \to x^*\text{)}$$

Note that

$$|x^{k+1} - x^*| \leq \underbrace{\frac{\alpha_1}{2\alpha_2}|x^k - x^*|}_{\text{required to be } <1} \ |x^k - x^*|$$

If $\frac{\alpha_1}{2\alpha_2}|x^k - x^*| < 1 \ \forall\ k$, then

$$|x^{k+1} - x^*| < |x^k - x^*| \ \forall\ k$$

How to choose α_1 and α_2?
At $x^*, g(x^*) = 0$, and $g'(x^*) > 0$
Since $g' \in \mathcal{C}^0$, $\exists\ \eta > 0 \ \ni g'(x) > 0 \ \forall\ x \in (x^* - \eta, x^* + \eta)$
Let

$$\begin{aligned} \alpha_1 &= \max_{x \in (x^* - \eta, x^* + \eta)} |g''(x)| \\ \alpha_2 &= \min_{x \in (x^* - \eta, x^* + \eta)} g'(x) \end{aligned}$$

Therefore,

$$\left| \frac{1}{2} \frac{g''(\bar{x}^k)}{g'(x^k)} \right| \leq \frac{\alpha_1}{2\alpha_2} = \beta, \text{ say.}$$

Preferable to choose $x^0 \in (x^* - \eta, x^* + \eta)$

Also, we want $\beta|x^k - x^*| < 1 \; \forall \; k$. That is,

$$\begin{aligned} |x^k - x^*| &< 1/\beta \; \forall \; k \\ \Rightarrow \quad x^k &\in (x^* - 1/\beta, x^* + 1/\beta) \end{aligned}$$

Therefore, choose $x^0 \in (x^* - \eta, x^* + \eta) \cap (x^* - 1/\beta, x^* + 1/\beta)$

Does $\{x^k\}$ converge to x^* if x^0 is chosen using this approach?

We have

$$\begin{aligned} |x^k - x^*| &\leq \beta|x^{k-1} - x^*|^2 \\ \therefore \beta|x^k - x^*| &\leq (\beta|x^0 - x^*|)^{2^k} \\ \therefore |x^k - x^*| &\leq \frac{1}{\beta}(\underbrace{\beta|x^0 - x^*|}_{<1})^{2^k} \end{aligned}$$

Therefore,

$$\lim_{k \to \infty} |x^k - x^*| = 0$$

Not a practical approach to choose x^0

Theorem

Let $f : \mathbb{R} \rightarrow \mathbb{R}$, $f \in \mathcal{C}^3$. *Let* $x^* \in \mathbb{R}$ *be such that* $g(x^*) = 0$ *and* $g'(x^*) > 0$. *Then, provided* x^0 *is sufficiently close to* x^*, *the sequence* $\{x^k\}$ *generated by classical Newton algorithm converges to* x^* *with an order of convergence two.*

Initialization of x^0 requires knowledge of x^*!

Modified Newton Method

Modifications:

- Given $\boldsymbol{x}^k$ and $\boldsymbol{d}_N^k = -(\boldsymbol{H}^k)^{-1}\boldsymbol{g}^k$,
  Fix some constant $\delta > 0$.
  Find the smallest $\zeta_k \geq 0$ such that the smallest eigenvalue of the matrix $(\boldsymbol{H}^k + \zeta_k \boldsymbol{I})$ is greater than δ.
  Therefore, $\boldsymbol{d}^k = -(\boldsymbol{H}^k + \zeta_k \boldsymbol{I})^{-1}\boldsymbol{g}^k$ is a descent direction.
- Given $\boldsymbol{x}^k$ and $\boldsymbol{d}^k = -(\boldsymbol{H}^k + \zeta_k \boldsymbol{I})^{-1}\boldsymbol{g}^k$, use line search techniques to determine α^k and $\boldsymbol{x}^{k+1}$

$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \alpha^k \boldsymbol{d}^k$$

Modified Newton Algorithm

(1) Initialize $\boldsymbol{x}^0$, ϵ and δ, set $k := 0$.

(2) **while** $\|\boldsymbol{g}^k\| > \epsilon$

  (a) Find the smallest $\zeta_k \geq 0$ such that the smallest eigenvalue of $\boldsymbol{H}^k + \zeta_k \boldsymbol{I}$ is greater than δ

  (b) Set $\boldsymbol{d}^k = -(\boldsymbol{H}^k + \zeta_k \boldsymbol{I})^{-1} \boldsymbol{g}^k$

  (c) Find $\alpha^k (> 0)$ along $\boldsymbol{d}^k$ such that

    (i) $f(\boldsymbol{x}^k + \alpha^k \boldsymbol{d}^k) < f(\boldsymbol{x}^k)$

    (ii) α^k satisfies Armijo-Wolfe (or Armijo-Goldstein) conditions

  (d) $\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \alpha^k \boldsymbol{d}^k$

  (e) $k := k + 1$

endwhile

Output : $\boldsymbol{x}^* = \boldsymbol{x}^k$, a stationary point of $f(\boldsymbol{x})$.

- Modified Newton algorithm has global convergence properties and has order of convergence equal to two