Constrained Optimization I

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Objective

At the end of this chapter you should be able to:

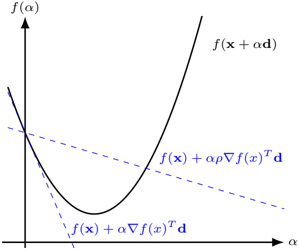
- Describe, implement, and the constrained optimization problems

Reviews: Back Tracking Line Search

- The **backtracking** line search is very simple and quite effective.
- Depend on two constants α, β with $0 < \beta < 0.5, 0 < \rho < 1$.

Require: a descent direction $\mathbf{d}$, $\beta \in (0, 0.5)$ and $\rho \in (0, 1)$

$\alpha = 1$
while $f(\mathbf{x} + \alpha\mathbf{d}) > f(\mathbf{x}) + \beta\alpha\nabla f(\mathbf{x})^T\mathbf{d}$ do
  $\alpha = \rho\alpha$
end while
return α



- The lower dashed line shows the linear extrapolation of $f(\mathbf{x})$
- The upper dashed line ahs a slope of a factor of ρ smaller.
- The backtracking condition is that $f(\mathbf{x})$ is lies below the upper dashed line.

Newton Method with Line Search

Minimizer of second-order approximation

$$f(\mathbf{x}+\Delta\mathbf{x}) \approx f(\mathbf{x}) + \nabla f(\mathbf{x})^T \Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^T \nabla^2 f(x) \Delta\mathbf{x}$$

$$\nabla f(\mathbf{x}+\Delta\mathbf{x}) = \nabla f(\mathbf{x}) + \nabla^2 f(x)\Delta\mathbf{x} = 0 \qquad \text{(with respect to } \Delta\mathbf{x})$$

The second equation is the optimality condition. We have

$$\Delta\mathbf{x} = -\nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x}) = \mathbf{d}$$

The positive definiteness of $\nabla^2 f(x)$ implies that

$$\nabla f(x)^T \Delta x = -\nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x) = -\mathbf{g}^T \mathbf{H}^{-1} \mathbf{g} < 0$$

The Newton step is a descent direction (unless $\mathbf{x}$ is optimal).

Newton Method with Line Search

- The local Newton method is

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x}_k)$$

- Newton method with line search

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{D}_k \nabla f(\mathbf{x}_k) = \mathbf{x}_k - \alpha_k \nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x}_k)$$

  In general the Hessian matrix $\nabla^2 f(\mathbf{x}_k)$ may not be positive definite, it is necessary to choose another preconditioner.

- One of then involves choosing $\mathbf{D}_k$ diagonal, with entries

$$\mathbf{D}_k(i,i) = \max\left(\varepsilon, \frac{\partial^2 f}{\partial(x)_i^2(\mathbf{x}_k)}\right)^{-1}$$

  with $\varepsilon > 0$. Then, each diagonal element (i.e., each eigenvalue) is greater than or equal to ε, which guarantees the positive definiteness of the matrix.

Newton Method with Line Search

Modified Cholesky factorization

Require: A symmetric matrix $A \in \mathbb{R}^{n \times n}$

$k = 0$

if $\min_i a_{ii} > 0$ **then**

  $\tau_k = 0$

else

  $\tau_k = \frac{1}{2}\|A\|_F$

end if

repeat

  Calculate the Cholesky factorization $\mathbf{L}\mathbf{L}^T$ of $A + \tau\mathbf{I}$

  if the factorization is not successful **then**

    $\tau_{k+1} = \max(2\tau_k, \frac{1}{2}\|A\|_F)$

    $k = k + 1$

  end if

until the factorization is successful

return τ_{k+1}

Newton Method with Line Search

- The most widely used technique is the regularization (damped Newton or Levenberg–Marquardt algorithm).

$$\mathbf{D}_k = \left(\nabla^2 f(\mathbf{x}_k) + \tau \mathbf{I}\right)^{-1}$$

Require: a starting point $\mathbf{x}$, tolerance $\varepsilon > 0$

$k = 0$

repeat

Calculate a lower triangular matrix $\mathbf{L}_k$ and τ such that

$\mathbf{L}_k \mathbf{L}_k^T = \nabla^2 f(\mathbf{x}_k) + \tau \mathbf{I}$

by using the modified Cholesky factorization

Find $\mathbf{z}_k$ by solving the triangular system $\mathbf{L}_k \mathbf{z}_k = \nabla f(\mathbf{x}_k)$

Find $\mathbf{d}_k$ by solving the triangular system $\mathbf{L}_k^T \mathbf{d}_k = -\mathbf{z}_k$

Choose step size α_k by backtracking line search with $\alpha_0 = 1$

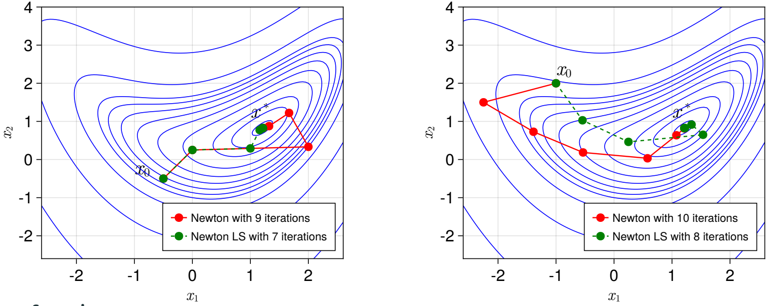
$x_{k+1} = x_k + \alpha_k \mathbf{d}_k$

$k = k + 1$

until $\|\nabla f(\mathbf{x}_k)^T \nabla^2 f(\mathbf{x}_k)^{-1} \nabla f(\mathbf{x}_k)\| \leq \varepsilon$

return x_{k+1}

Newton Method with Line Search



Bean function:

$$f(\mathbf{x}) = (1 - x_1)^2 + (1 - x_2)^2 + 0.5(2x_2 - x_1^2)^2$$

- The Newton decrement is that it is independent of linear changes in the problem variables.
- The backtracking line search especially suitable for a Newton algorithm is that as the iterates approach the solution proin, α_k approaches unity, the quadratic approximation used as the basis fo the newton method becomes increasingly accurate.

Equality Constrained Minimized

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} = \mathbf{b}, \end{aligned}$$

where $f(\mathbf{x})$ is a convex twice continuously differentiable function and $\mathbf{A}$ is of full row rank. The KKT condition is

$$\begin{aligned} \nabla f(\mathbf{x}) + \mathbf{A}^T \boldsymbol{\lambda} = 0 \\ \mathbf{A}\mathbf{x} = \mathbf{b} \end{aligned}$$

are satisfied for some Lagrange multiplier $\boldsymbol{\lambda}$.

- Assume $\mathbf{x}^*, \boldsymbol{\lambda}^*$ exist, then $\mathbf{x}_k, \boldsymbol{\lambda}_k$ satisfies $\mathbf{A}\mathbf{x} = \mathbf{b}$.

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + \mathbf{d}_k \\ \mathbf{A}\mathbf{x}_{k+1} &= \mathbf{A}\mathbf{x}_k + \mathbf{A}\mathbf{d}_k \quad \Rightarrow \quad \mathbf{A}\mathbf{d}_k = 0 \end{aligned}$$

Equality Constrained Minimized

- The linear approximation of the gradient is

$$\begin{aligned} \nabla f(\mathbf{x}_k + \mathbf{d}_k) &\approx \nabla f(\mathbf{x}_k) + \nabla^2 f(\mathbf{x}_k)\mathbf{d}_k \\ &= \nabla f(\mathbf{x}_k) + \mathbf{H}_k \mathbf{d}_k \end{aligned}$$

- KKT Condition becomes

$$\begin{aligned} \nabla f(\mathbf{x}_k) + \nabla^2 f(\mathbf{x}_k)\mathbf{d}_k + \mathbf{A}^T \boldsymbol{\lambda}_{k+1} &= 0 \\ \mathbf{A}\mathbf{d}_k &= 0 \end{aligned}$$

- Matrix Form:

$$\begin{bmatrix} \nabla^2 f(\mathbf{x}_k) & \mathbf{A}^T \\ \mathbf{A} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{d}_k \\ \boldsymbol{\lambda}_{k+1} \end{bmatrix} = \begin{bmatrix} -\nabla f(\mathbf{x}_k) \\ 0 \end{bmatrix}$$

Equality Constrained Minimized

- If there are no constraints, it becomes

$$\begin{aligned} \mathbf{H}_k \mathbf{d}_k &= -\nabla f(\mathbf{x}) \\ \mathbf{d}_k &= -\mathbf{H}_k^{-1} \nabla f(\mathbf{x}) \end{aligned}$$

The vector $\mathbf{d}_k$ satisfies the constraints is regarded as a Newton direction.

- We can calculate $\mathbf{d}_k$ as

$$\mathbf{d}_k = -\mathbf{H}_k^{-1} \left(\mathbf{A}^T \boldsymbol{\lambda}_{k+1} + \nabla f(\mathbf{x}_k) \right)$$

where

$$\begin{aligned} \mathbf{d}_k &= -\mathbf{H}_k^{-1} \mathbf{A}^T \boldsymbol{\lambda}_{k+1} - \mathbf{H}_k^{-1} \nabla f(\mathbf{x}_k) \\ \boldsymbol{\lambda}_{k+1} &= -\left(\mathbf{A} \mathbf{H}_k^{-1} \mathbf{A}^T \right) \mathbf{A} \mathbf{H}_k^{-1} \nabla f(\mathbf{x}_k) \\ \mathbf{A} \mathbf{d}_k &= 0 \end{aligned}$$

- The stop criterion can be formulate as $\|\nabla f(\mathbf{x}_{k+1}) + \mathbf{A}^T \boldsymbol{\lambda}_{k+1}\| < \varepsilon$

Equality Constrained Minimized

Newton Method with Linear Constraints and $\mathbf{x} \in$ dom $f(\mathbf{x})$

Require: a starting point $\mathbf{x} \in$ dom $f(\mathbf{x})$, $\boldsymbol{\lambda}$, tolerance $\varepsilon > 0$
$k = 0$
repeat
Calculate $\mathbf{d}_k$ and $\boldsymbol{\delta}_k$
Find α_k that $\min\text{imize} \quad f(\mathbf{x}_k + \alpha\mathbf{d}_k)$, using the backtracking line search
$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k\mathbf{d}_k$ and compute $\nabla f(\mathbf{x}_{k+1})$
$k = k + 1$
until $\|\nabla f(\mathbf{x}_{k+1}) + \mathbf{A}^T\boldsymbol{\lambda}_{k+1}\| \leq \varepsilon$
return x_{k+1}

Equality Constrained Minimized

- If $\mathbf{x}$ is not in **dom** $f(\mathbf{x})$, $(\mathbf{x}_k, \boldsymbol{\lambda}_k)$ is known but $\mathbf{x}_k$ is not feasible

$$(\mathbf{x}_k, \boldsymbol{\lambda}_k) \quad \rightarrow \quad (\mathbf{x}_{k+1}, \boldsymbol{\lambda}_{k+1})$$

  We must have $\mathbf{A}\mathbf{d}_k = 0 = -(\mathbf{A}\mathbf{x} - b)$

- The Newton direction must satisfy the equations:

$$\begin{bmatrix} \mathbf{H}_k & \mathbf{A}^T \\ \mathbf{A} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{d}_k \\ \boldsymbol{\lambda}_{k+1} \end{bmatrix} = \begin{bmatrix} -\nabla f(\mathbf{x}_k) \\ \mathbf{b} - \mathbf{A}\mathbf{x}_k \end{bmatrix}$$

- Here $\mathbf{A}\mathbf{d}_k \neq 0$ $\mathbf{d}_k$ is not necessarily a descent direction. The line search and the stop criterion are not applicable.
- Let use $\boldsymbol{\lambda}_{k+1} = \boldsymbol{\lambda}_k + \boldsymbol{\delta}_k$

$$\begin{bmatrix} \mathbf{H} & \mathbf{A}^T \\ \mathbf{A} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{d}_k \\ \boldsymbol{\delta}_k \end{bmatrix} = - \begin{bmatrix} \mathbf{r}_d \\ \mathbf{r}_p \end{bmatrix}$$

Equality Constrained Minimized

- $\mathbf{r}_d$ and $\mathbf{r}_p$ is called **dual** and **primal residual**

$$\mathbf{r}_d = \nabla f(\mathbf{x}_k) + \mathbf{A}^T \boldsymbol{\lambda}_k$$
$$\mathbf{r}_p = \mathbf{A}\mathbf{x}_k - \mathbf{b}$$

- We have

$$\mathbf{d}_k = -\mathbf{H}_k^{-1}\left(\mathbf{A}^T\boldsymbol{\delta}_k + \mathbf{r}_d\right)$$
$$\boldsymbol{\delta}_k = -\left(\mathbf{A}\mathbf{H}_k^{-1}\mathbf{A}^T\right)^{-1}\left(\mathbf{A}\mathbf{H}_k^{-1}\mathbf{r}_d - \mathbf{r}_p\right)$$

$$\|\mathbf{r}(\mathbf{x}_k, \boldsymbol{\lambda}_k)\| \le \varepsilon$$

- The backtracking line search can be found by

$$\text{minimize}\, \|\mathbf{r}(\mathbf{x}_k + \alpha_k\mathbf{d}_k, \boldsymbol{\lambda}_k + \alpha_k\boldsymbol{\delta}_k\|$$

Equality Constrained Minimized

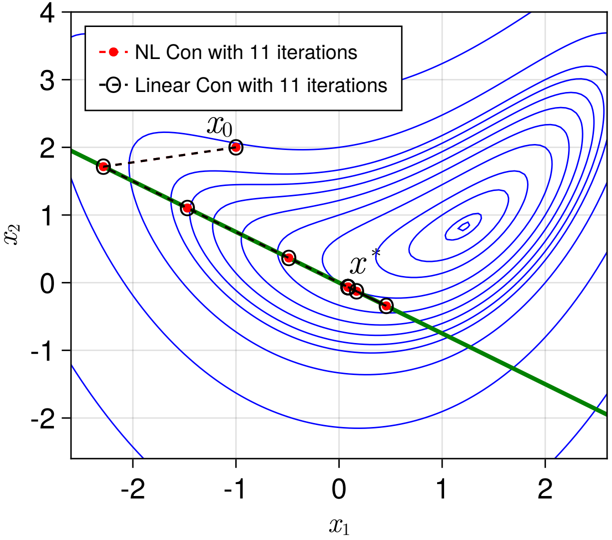
Newton Method with Linear Constraints and $\mathbf{x}$ is not in dom $f(\mathbf{x})$

Require: a starting point $\mathbf{x}, \boldsymbol{\lambda}$, tolerance $\varepsilon > 0$
  $k = 0$
  repeat
    Calculate $\mathbf{d}_k$ and $\boldsymbol{\lambda}_{k+1}$
    Find α_k using backtracking that minimizes $\|\mathbf{r}(\mathbf{x}_k + \alpha\mathbf{d}_k, \boldsymbol{\lambda}_k + \alpha\boldsymbol{\delta}_k)\|$
    $x_{k+1} = x_k + \alpha_k\mathbf{d}_k$
    $k = k + 1$
  until $\|\mathbf{r}(\mathbf{x}_k, \boldsymbol{\lambda}_k)\| < \varepsilon$
  return x_{k+1}

Modified Backtracking

Require: $\gamma \in (0, 0.5)$ and $\rho \in (0, 1)$, $\lambda = 1$
  while $\|\mathbf{r}(\mathbf{x}_k + \alpha\mathbf{d}_k, \boldsymbol{\lambda}_k + \alpha\boldsymbol{\delta}_k\| > (1 - \rho\alpha)\|\mathbf{r}(\mathbf{x}_k, \boldsymbol{\lambda}_k)\|$ **do**
    $\alpha = \gamma\alpha$
  end while
  return x_{k+1}

Equality Constrained Minimized



Nonlinear Equality Constrained Minimized

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & f(\mathbf{x}), \qquad f(\mathbf{x}) : \mathbb{R}^n \mapsto \mathbb{R} \\ \text{subject to} \quad & c(\mathbf{x}) = 0, \qquad c(\mathbf{x}) : \mathbb{R}^n \mapsto \mathbb{R}^m \end{aligned}$$

First-Order Necessary Conditions:

- $\nabla f(\mathbf{x}) = 0$ in free directions
- $c(\mathbf{x}) = 0$ for active constraints.
- Any non-zero component of $\nabla f(\mathbf{x})$ must be normal to the constraint surface/manifold

$$\nabla f(\mathbf{x}) + \lambda \nabla c(\mathbf{x}) = 0,$$

where λ is a Lagrange multiplier(dual variable).

Nonlinear Equality Constrained Minimized

- In general

$$\frac{\partial f}{\partial \mathbf{x}} + \boldsymbol{\lambda}^T \frac{\partial c}{\partial \mathbf{x}} = 0, \qquad \boldsymbol{\lambda} \in \mathbb{R}^m$$

- Based on this gradient condition, we defined:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \boldsymbol{\lambda}^T c(\mathbf{x}),$$

  where $\mathcal{L}$ is called "Lagrangian"
- The KKT condition is

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = \nabla f(\mathbf{x}) + \left(\frac{\partial c}{\partial \mathbf{x}}\right)^T \boldsymbol{\lambda} = 0$$

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = c(\mathbf{x}) = 0$$

Nonlinear Equality Constrained Minimized

We can solve the KKT condition with the Newton method:

$$\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x}+\Delta\mathbf{x},\boldsymbol{\lambda}+\Delta\boldsymbol{\lambda}) \approx \nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x},\boldsymbol{\lambda}) + \frac{\partial^2\mathcal{L}}{\partial\mathbf{x}^2}\Delta\mathbf{x} + \frac{\partial^2\mathcal{L}}{\partial\mathbf{x}\partial\boldsymbol{\lambda}}\Delta\boldsymbol{\lambda} = 0$$

$$\nabla_{\boldsymbol{\lambda}}\mathcal{L}(\mathbf{x}+\Delta\mathbf{x},\boldsymbol{\lambda}+\Delta\boldsymbol{\lambda}) \approx c(\mathbf{x}) + \frac{\partial c}{\partial\boldsymbol{\lambda}}\Delta\mathbf{x} = 0$$

Note:

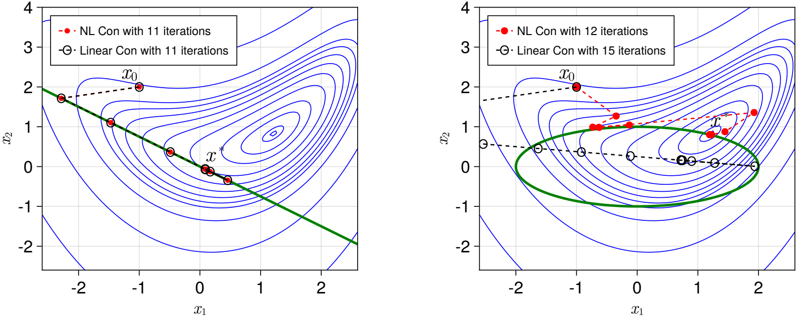
$$\frac{\partial}{\partial\mathbf{x}}\nabla_{\boldsymbol{\lambda}}\mathcal{L}(\mathbf{x},\boldsymbol{\lambda}) = \left(\frac{\partial c}{\partial\mathbf{x}}\right)^T, \qquad \frac{\partial c}{\partial\mathbf{x}}\Delta\mathbf{x} = -c(\mathbf{x})$$

The KKT system is

$$\begin{bmatrix} \frac{\partial^2\mathcal{L}}{\partial\mathbf{x}^2} & \left(\frac{\partial c}{\partial\mathbf{x}}\right)^T \\ \frac{\partial c}{\partial\boldsymbol{\lambda}} & 0 \end{bmatrix} \begin{bmatrix} \Delta\mathbf{x} \\ \Delta\boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} -\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x},\boldsymbol{\lambda}) \\ -c(\mathbf{x}) \end{bmatrix}$$

In the algorithm we have $\mathbf{x}_{k+1} = \mathbf{x}_k + \Delta\mathbf{x}$ and $\boldsymbol{\lambda}_{k+1} = \boldsymbol{\lambda}_k + \Delta\boldsymbol{\lambda}$.

Nonlinear Equality Constrained Minimized



When the equality constraints are nonlinear, it is obvious that the Newton with Linear constraint method cannot use.

Reference

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