Numerical Optimization

Unit 9: Penalty Method and Interior Point Method
Unit 10: Filter Method and the Maratos Effect

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Penalty method

- The idea is to add penalty terms to the objective function, which turns a constrained optimization problem to an unconstrained one.

Quadratic penalty function

Example (For equality constraints)

$\min x_1 + x_2$ subject to $x_1^2 + x_2^2 - 2 = 0 \qquad (\vec{x}^* = (1,1))$

$\Rightarrow$ Define $Q(\vec{x},\mu) = x_1 + x_2 + \dfrac{\mu}{2}(x_1^2 + x_2^2 - 2)^2$

For $\mu = 1$,

$$\nabla Q(\vec{x},1) = \begin{pmatrix} 1 + 2(x_1^2 + x_2^2 - 2)x_1 \\ 1 + 2(x_1^2 + x_2^2 - 2)x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \vec{x}_1^* \\ \vec{x}_2^* \end{pmatrix} = \begin{pmatrix} -1.1 \\ -1.1 \end{pmatrix}$$

For $\mu = 10$,

$$\nabla Q(\vec{x},10) = \begin{pmatrix} 1 + 20(x_1^2 + x_2^2 - 2)x_1 \\ 1 + 20(x_1^2 + x_2^2 - 2)x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \vec{x}_1^* \\ \vec{x}_2^* \end{pmatrix} = \begin{pmatrix} -1.0000001 \\ -1.0000001 \end{pmatrix}$$

Size of μ

- It seems the larger μ, the better solution is.
- When μ is large, matrix $\nabla^2 Q \approx \mu \nabla c \nabla c^T$ is ill-conditioned.

$$Q(x, \mu) = f(x) + \frac{\mu}{2}(c(x))^2$$

$$\nabla Q = \nabla f + \mu c \nabla c$$

$$\nabla^2 Q = \nabla^2 f + \mu \nabla c \nabla c^T + \mu c \nabla^2 c$$

- μ cannot be too small either.

Example

$\min_{\vec{x}} -5x_1^2 + x_2^2$ s.t. $x_1 = 1$.

$Q(\vec{x}, \mu) = -5x_1^2 + x_2^2 + \frac{\mu}{2}(x_1 - 1)^2$.

For $\mu < 10$, the problem $\min Q(\vec{x}, \mu)$ is unbounded.

Quadratic penalty function

- Picks a proper initial guess of μ and gradually increases it.

Algorithm: Quadratic penalty function

1. Given $\mu_0 > 0$ and $\vec{x}_0$
2. For $k = 0, 1, 2, \ldots$
    1. Solve $\min_{\vec{x}} Q(:, \mu_k) = f(\vec{x}) + \frac{\mu_k}{2} \sum_{i \in \mathbb{E}} c_i^2(\vec{x})$.
    2. If converged, stop
    3. Increase $\mu_{k+1} > \mu_k$ and find a new x_{k+1}

- Problem: the solution is not exact for $\mu \leq \infty$.

Augmented Lagrangian method

- Use the Lagrangian function to rescue the inexactness problem.
- Let

$$\mathcal{L}(\vec{x},\vec{\rho},\mu) = f(\vec{x}) - \sum_{i\in\varepsilon} \rho_i c_i(\vec{x}) + \frac{\mu}{2}\sum_{i\in\varepsilon} c_i^2(\vec{x})$$

$$\nabla\mathcal{L} = \nabla f(\vec{x}) - \sum_{i\in\varepsilon} \rho_i \nabla c_i(\vec{x}) + \mu \sum_{i\in\varepsilon} c_i(\vec{x})\nabla c_i.$$

- By the Lagrangian theory, $\nabla\mathcal{L} = \nabla f - \sum_{i\in\varepsilon} \underbrace{(\rho_i - \mu c_i)}_{\lambda_i^*} \nabla c_i$.
- At the optimal solution, $c_i(\vec{x}^*) = \dfrac{-1}{\mu}(\lambda_i^* - \rho_i)$.
- If we can approximate $\rho_i \longrightarrow \lambda_i^*$, μ_k need not be increased indefinitely,

$$\lambda_i^{k+1} = \lambda_i^k - \mu_k c_i(x_k)$$

- Algorithm: update ρ_i at each iteration.

Inequality constraints

There are two approaches to handle inequality constraints.

1. Make the object function nonsmooth (non-differentiable at some points).
2. Add slack variable to turn the inequality constraints to equality constraints.

$$c_i \geq 0 \Rightarrow \begin{cases} c_i(\vec{x}) - s_i = 0 \\ s_i \geq 0 \end{cases}$$

   - But then we have bounded constraints for slack variables.

We will focus on the second approach here.

Inequality constraints

- Suppose the augmented Lagrangian method is used and all inequality constraints are converted to bounded constraints.
- For a fixed μ and $\vec{\lambda}$,

$$\begin{array}{ll} \min\limits_{\vec{x}} & \mathcal{L}(\vec{x}, \vec{\lambda}, \mu) = f(\vec{x}) - \sum_{i=1}^{m} \lambda_i c_i(\vec{x}) + \frac{\mu}{2} \sum_{i=1}^{m} c_i^2(\vec{x}) \\ \text{s.t.} & \vec{\ell} \leq \vec{x} \leq \vec{u} \end{array}$$

- The first order necessary condition for $\vec{x}$ to be a solution of the above problem is

$$\vec{x} = P(\vec{x} - \nabla_x \mathcal{L}_A(\vec{x}, \vec{\lambda}, \mu), \vec{\ell}, \vec{u}),$$

where

$$P(\vec{g}, \vec{\ell}, \vec{u}) = \begin{cases} \ell_i, & \text{if } g_i \leq \ell_i; \\ g_i, & \text{if } g_i \in (\ell_i, u_i); \\ u_i, & \text{if } g_i \geq u_i. \end{cases} \qquad \text{for all } i = 1, 2, \ldots, n.$$

Nonlinear gradient projection method

Sequential quadratic programming + trust region method to solve

$$\min_{\vec{x}} f(\vec{x}) \qquad \text{s.t.} \quad \vec{\ell} \le \vec{x} \le \vec{u}$$

Algorithm: Nonlinear gradient projection method

1. At each iteration, build a quadratic model

$$q(\vec{x}) = \frac{1}{2}(x - x_k)^T B_k (x - x_k) + \nabla f_k^T (x - x_k)$$

   where B_k is SPD approximation of $\nabla^2 f(x_k)$.

2. For some Δ_k, use the gradient projection method to solve

$$\begin{array}{ll} \min\limits_{\vec{x}} & q(\vec{x}) \\ \text{s.t.} & \max(\vec{\ell}, \vec{x}_k - \Delta_k) \le \vec{x} \le \max(\vec{u}, \vec{x}_k + \Delta_k), \end{array}$$

3. Update Δ_k and repeat 1-3 until converge.

Interior point method

- Consider the problem

$$
\begin{array}{ll}
\min_{\vec{x}} & f(\vec{x}) \\
\text{s.t.} & \quad C_E(\vec{x}) = 0 \\
 & \quad C_I(\vec{x}) - \vec{s} = 0 \\
 & \quad \vec{s} \geq 0
\end{array}
$$

  where $\vec{s}$ are slack variables.
- The interior point method starts a point inside the feasible region, and builds "walls" on the boundary of the feasible region.
- A barrier function goes to infinity when the input is close to zero.

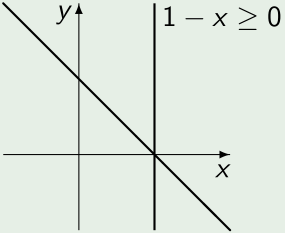
$$
\min_{\vec{x},\vec{s}} f(\vec{x}) - \mu \sum_{i=1}^{m} \log(s_i) \text{ s.t. } \begin{array}{l} C_E(\vec{x}) = 0 \\ C_I(\vec{x}) - \vec{s} = 0 \end{array} \tag{1}
$$

  - The function $f(x) = -\log x \to \infty$ as $x \to 0$.
  - μ: barrier parameter

An example

Example ($\min -x+1$, s.t. $x \le 1$)

$\min_{\vec{x}} -x + 1 - \mu \ln(1-x)$



$$
\begin{aligned}
\mu &= 1, & x^* &= 0.00005 \\
\mu &= 0.1, & x^* &= 0.89999 \\
\mu &= 0.01, & x^* &= 0.989999 \\
\mu &= 10^{-5}, & x^* &= 0.99993
\end{aligned}
$$

- The Lagrangian of (1) is

$$\mathcal{L}(\vec{x}, \vec{s}, \vec{y}, \vec{z}) = f(\vec{x}) - \mu \sum_{i=1}^{m} \log(s_i) - \vec{y}^T C_E(\vec{x}) - \vec{z}^T (C_I(\vec{x}) - \vec{s})$$

1. Vector $\vec{y}$ is the Lagrangian multiplier of equality constraints.
2. Vector $\vec{z}$ is the Lagrangian multiplier of inequality constraints.

The KKT conditions

The KKT conditions

The KKT conditions for (1)

$$\begin{array}{rrl} \nabla_x \mathcal{L} = 0 \Rightarrow & \nabla f - A_E \vec{y} - A_I \vec{z} & = 0 \\ \nabla_s \mathcal{L} = 0 \Rightarrow & SZ - \mu I & = 0 \\ \nabla_y \mathcal{L} = 0 \Rightarrow & C_E(\vec{x}) & = 0 \\ \nabla_z \mathcal{L} = 0 \Rightarrow & C_I(\vec{x}) - \vec{s} & = 0 \end{array} \tag{2}$$

- Matrix $S = \mathrm{diag}(\vec{s})$ and matrix $Z = \mathrm{diag}(\vec{z})$.
- Matrix A_E is the Jacobian of C_E and matrix A_I is the Jacobian of C_I.

Newton's step

Let $F = \begin{pmatrix} \nabla_x \mathcal{L} \\ \nabla_s \mathcal{L} \\ \nabla_y \mathcal{L} \\ \nabla_z \mathcal{L} \end{pmatrix} = \begin{pmatrix} \nabla f - A_E \vec{y} - A_I \vec{z} \\ SZ - \mu I \\ C_E(\vec{x}) \\ C_I(\vec{x}) - \vec{s} \end{pmatrix}.$

The interior point method uses Newton's method to solve $F = 0$.

$$\nabla F = \begin{bmatrix} \nabla_{xx}\mathcal{L} & 0 & -A_E(\vec{x}) & -A_I(\vec{x}) \\ 0 & Z & 0 & S \\ A_E(\vec{x}) & 0 & 0 & 0 \\ A_I(\vec{x}) & -I & 0 & 0 \end{bmatrix}$$

Newton's step

$$\nabla F = \begin{pmatrix} \vec{p}_x \\ \vec{p}_s \\ \vec{p}_y \\ \vec{p}_z \end{pmatrix} = -F \qquad \begin{aligned} \vec{x}_{k+1} &= \vec{x}_k + \alpha_x \vec{p}_x \\ \vec{s}_{k+1} &= \vec{s}_k + \alpha_s \vec{p}_s \\ \vec{y}_{k+1} &= \vec{y}_k + \alpha_y \vec{p}_y \\ \vec{z}_{k+1} &= \vec{z}_k + \alpha_z \vec{p}_z \end{aligned}$$

Algorithm: Interior point method (IPM)

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1. Given initial $\vec{x}_0, \vec{s}_0, \vec{y}_0, \vec{z}_0$, and μ_0
2. For $k = 0, 1, 2, \ldots$ until converge
   (a) Compute $\vec{p}_x, \vec{p}_s, \vec{p}_y, \vec{p}_z$ and $\alpha_x, \alpha_s, \alpha_y, \alpha_z$
   (b) $(\vec{x}_{k+1}, \vec{s}_{k+1}, \vec{y}_{k+1}, \vec{z}_{k+1}) = (\vec{x}_k, \vec{s}_k, \vec{y}_k, \vec{z}_k) + (\alpha_x \vec{p}_x, \alpha_s \vec{p}_s, \alpha_y \vec{p}_y, \alpha_z \vec{p}_z)$
   (c) Adjust $\mu_{k+1} < \mu_k$

Some comments of the interior point method

1. The complementarity slackness condition says $s_i z_i = 0$ at the optimal solution, by which, the parameter μ, $SZ = \mu I$, needs to decrease to zero as the current solution approaches to the optimal solution.
2. Why cannot we set μ zero or small in the beginning? Because that will make $\vec{x}_k$ going to the nearest constraint, and the entire process will move along constraint by constraint, which again becomes an exponential algorithm.
3. To keep $\vec{x}_k$ (or $\vec{s}$ and $\vec{z}$) too close any constraints, IPM also limits the step size of $\vec{s}$ and $\vec{z}$

$$
\begin{aligned}
\alpha_s^{\max} &= \max\{\alpha \in (0,1], \vec{s} + \alpha \vec{p}_s \geq (1-\tau)\vec{s}\} \\
\alpha_z^{\max} &= \max\{\alpha \in (0,1], \vec{z} + \alpha \vec{p}_z \geq (1-\tau)\vec{z}\}
\end{aligned}
$$

Interior point method for linear programming

- We will use linear programming to illustrate the details of IPM.

The primal	The dual
$\min_{\vec{x}} \ \vec{c}^T\vec{x}$ s.t. $A\vec{x} = \vec{b}$, $\vec{x} \geq 0$.	$\max_{\vec{\lambda}} \ \vec{b}^T\vec{\lambda}$ s.t. $A^T\vec{\lambda} + \vec{s} = \vec{c}$, $\vec{s} \geq 0$.

- KKT conditions

$$
\begin{aligned}
A^T\vec{\lambda} + \vec{s} &= \vec{c} \\
A\vec{x} &= \vec{b} \\
x_i s_i &= 0 \\
\vec{x} \geq 0, \vec{s} &\geq 0
\end{aligned}
$$

Solve problem

Let $X = \begin{pmatrix} x_1 & & & \\ & x_2 & & \\ & & \ddots & \\ & & & x_n \end{pmatrix}, S = \begin{pmatrix} s_1 & & & \\ & s_2 & & \\ & & \ddots & \\ & & & s_n \end{pmatrix},$

$F = \begin{bmatrix} A^T\vec{\lambda} + \vec{s} - \vec{c} \\ A\vec{x} - \vec{b} \\ X\vec{s} - \mu\vec{e} \end{bmatrix}$

- The problem is to solve $F = 0$

Newton's method

Using Newton's method

$$\nabla F = \begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S & 0 & X \end{bmatrix}$$

$$\nabla F \begin{bmatrix} \vec{p}_x \\ \vec{p}_\lambda \\ \vec{p}_z \end{bmatrix} = -F \qquad \begin{aligned} \vec{x}_{k+1} &= \vec{x}_k + \alpha_x \vec{p}_x \\ \vec{\lambda}_{k+1} &= \vec{\lambda}_k + \alpha_\lambda \vec{p}_\lambda \\ \vec{z}_{k+1} &= \vec{z}_k + \alpha_z \vec{p}_z \end{aligned}$$

- How to decide μ_k?
  - $\mu_k = \frac{1}{n}\vec{x}_k . * \vec{s}_k$ is called duality measure.

The central path

The central path

- The central path: a set of points, $p(\tau) = \begin{pmatrix} x_\tau \\ \lambda_\tau \\ z_\tau \end{pmatrix}$, defined by the solution of the equation

$$\begin{aligned} A^T\vec{\lambda} + \vec{s} &= \vec{c} \\ A\vec{x} &= \vec{b} \\ x_i s_i &= \tau \qquad i = 1, 2, \cdots, n \\ \vec{x}, \vec{s} &> 0 \end{aligned}$$

Algorithm: The interior point method for solving linear programming

1. Given an interior point $\vec{x}_0$ and the initial guess of slack variables $\vec{s}_0$
2. For $k = 0, 1, \ldots$
   (a) Solve $\begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S^k & 0 & X^k \end{pmatrix} \begin{pmatrix} \Delta x_k \\ \Delta \lambda_k \\ \Delta s_k \end{pmatrix} = \begin{pmatrix} \vec{b} - A\vec{x}_k \\ \vec{c} - \vec{s}_k - A^T \vec{\lambda}_k \\ -X^k S^k e + \sigma_k \mu_k e \end{pmatrix}$ for $\sigma_k \in [0, 1]$.
   (b) Compute $(\alpha_x, \alpha_\lambda, \alpha_s)$ s.t. $\begin{pmatrix} \vec{x}_{k+1} \\ \vec{\lambda}_{k+1} \\ \vec{s}_{k+1} \end{pmatrix} = \begin{pmatrix} \vec{x}_k + \alpha_x \Delta x_k \\ \vec{\lambda}_k + \alpha_\lambda \Delta \lambda_k \\ \vec{s}_k + \alpha_s \Delta s_k \end{pmatrix}$ is in the neighborhood of the central path
   $$\mathcal{N}(\theta) = \left\{ \begin{pmatrix} \vec{x} \\ \vec{\lambda} \\ \vec{s} \end{pmatrix} \in \mathcal{F} \;\middle|\; \|XS\vec{e} - \mu\vec{e}\| \leq \theta\mu \right\} \text{ for some } \theta \in (0, 1].$$

Filter method

- There are two goals of constrained optimization:
  1. Minimize the objective function.
  2. Satisfy the constraints.

Example

Suppose the problem is

$$\begin{array}{lll} \min_{\vec{x}} & f(\vec{x}) & \\ \text{s.t.} & c_i(\vec{x}) = 0 & \text{for } i \in \mathcal{E} \\ & c_i(\vec{x}) \geq 0 & \text{for } i \in \mathcal{I} \end{array}$$

- Define $h(\vec{x})$ penalty functions of constraints.

$$h(\vec{x}) = \sum_{i \in \mathcal{E}} |c_i(\vec{x})| + \sum_{i \in \mathcal{I}} [c_i(\vec{x})]^-,$$

  in which the notation $[z]^- = \max\{0, -z\}$.
- The goals become $\begin{cases} \min f(\vec{x}) \\ \min h(\vec{x}) \end{cases}$

The filter method

- A pair (f_k, h_k) dominates (f_l, h_l) if $f_k < f_l$ and $h_k < h_l$.
- A filter is a list of pairs (f_k, h_k) such that no pair dominates any other.
- The filter method only accepts the steps that are not dominated by other pairs.

Algorithm: The filter method

1. Given initial $\vec{x}_0$ and an initial trust region Δ_0.
2. For $k = 0, 1, 2, \ldots$ until converge
   1. Compute a trial $\vec{x}^+$ by solving a local quadric programming model
   2. If (f^+, h^+) is accepted to the filter
      - Set $\vec{x}_{k+1} = \vec{x}^+$, add (f^+, h^+) to the filter, and remove pairs dominated by it.

      Else
      - Set $\vec{x}_{k+1} = \vec{x}_k$ and decrease Δ_k.

The Maratos effect

- The Maratos effect shows the filter method could reject a good step.

Example

$$\min_{x_1,x_2} f(x_1,x_2) = 2(x_1^2 + x_2^2 - 1) - x_1$$
$$\text{s.t. } x_1^2 + x_2^2 - 1 = 0$$

- The optimal solution is $\vec{x}^* = (1,0)$
- Suppose $\vec{x}_k = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \vec{p}_k = \begin{pmatrix} \sin^2\theta \\ -\sin\theta\cos\theta \end{pmatrix}$

$$\vec{x}_{k+1} = \vec{x}_k + \vec{p}_k = \begin{pmatrix} \cos\theta + \sin^2\theta \\ \sin\theta(1-\cos\theta) \end{pmatrix}$$

Reject a good step

- $\|\vec{x}_k - \vec{x}^*\| = \left\| \begin{pmatrix} \cos\theta - 1 \\ \sin\theta \end{pmatrix} \right\|$
  $= \sqrt{\cos^2\theta - 2\cos\theta + 1 + \sin^2\theta} = \sqrt{2(1-\cos\theta)}$
- $\|\vec{x}_{k+1} - \vec{x}^*\|$
  $= \left\| \begin{matrix} \cos\theta + \sin^2\theta - 1 \\ \sin\theta - \sin\theta\cos\theta \end{matrix} \right\| = \left\| \begin{matrix} \cos\theta(1-\cos\theta) \\ \sin\theta(1-\cos\theta) \end{matrix} \right\|$
  $= \sqrt{\cos^2\theta(1-\cos\theta)^2 + \sin^2\theta(1-\cos\theta)^2} = \sqrt{(1-\cos\theta)^2}$
- Therefore $\dfrac{\|\vec{x}_{k+1} - \vec{x}^*\|}{\|\vec{x}_k - \vec{x}^*\|^2} = \dfrac{1}{2}$. This step gives a quadratic convergence.
- However, the filter method will reject this step because

$$f(\vec{x}_k) = -\cos\theta, \text{ and } c(\vec{x}_k) = 0,$$

$$f(\vec{x}_{k+1}) = -\cos\theta - \sin 2\theta = \sin^2\theta - \cos\theta > f(\vec{x}_k)$$

$$c(\vec{x}_{k+1}) = \sin^2\theta > 0 = c(\vec{x}_k)$$

The second order correction

The second order correction could help to solve this problem.

- Instead of $\nabla c(\vec{x}_k)^T \vec{p}_k + c(\vec{x}_k) = 0$, use quadratic approximation

$$c(\vec{x}_k) + \nabla c(\vec{x}_k)^T \vec{d}_k + \frac{1}{2}\vec{d}_k^T \nabla^2_{xx} c(\vec{x})\vec{d}_k = 0. \tag{3}$$

- Suppose $\|\vec{d}_k - \vec{p}_k\|$ is small. Use Taylor expansion to approximate quadratic term

$$c(\vec{x}_k + \vec{p}_k) \approx c(\vec{x}_k) + \nabla c(\vec{x}_k)^T \vec{p}_k + \frac{1}{2}\vec{p}_k^T \nabla^2_{xx} c(\vec{x})\vec{p}_k.$$

$$\frac{1}{2}\vec{d}_k^T \nabla^2_{xx} c(\vec{x})\vec{d}_k \approx \frac{1}{2}\vec{p}_k^T \nabla^2_{xx} c(\vec{x})\vec{p}_k \approx c(\vec{x}_k + \vec{p}_k) - c(\vec{x}_k) - \nabla c(\vec{x}_k)^T \vec{p}_k.$$

- Equation (3) can be rewritten as

$$\nabla c(\vec{x}_k)^T \vec{d}_k + c(\vec{x}_k + \vec{p}_k) - \nabla c(\vec{x}_k)^T \vec{p}_k = 0$$

- Use the corrected linearized constraint:
  $\nabla c(\vec{x}_k)^T \vec{p} + c(\vec{x}_k + \vec{p}_k) - \nabla c(\vec{x}_k)^T \vec{p}_k = 0.$
  (The original linearized constraint is $\nabla c(\vec{x}_k)^T \vec{p} + c(\vec{x}_k) = 0$.)