10.34: Numerical Methods Applied to Chemical Engineering

Lecture 12:
Constrained Optimization
Equality constraints and Lagrange multipliers
Recap

- Unconstrained optimization
- Newton-Raphson methods
- Trust-region methods
Midterm Exam

• Expect 3 problems
• Comprehensive exam:
  • Linear algebra
  • Systems of nonlinear equations
  • Optimization
Constrained Optimization

- Problems of the sort:

\[
\min_{x \in D} f(x) \quad \text{arg min}_{x \in D} f(x)
\]

\[
f(x_1, x_2)
\]
Constrained Optimization

• Problems of the sort:

\[
\min_{x \in D} f(x) \quad \arg \min_{x \in D} f(x)
\]

• The feasible set can be described in terms of two types of constraints:
  
  • Equality constraints: \( \mathcal{D} = \{ x : c(x) = 0 \} \)
  
  • Inequality constraints: \( \mathcal{D} = \{ x : h(x) \geq 0 \} \)
Constrained Optimization

- Problems of the sort:

$$\min_{x \in D} f(x) \quad \arg \min_{x \in D} f(x)$$
Constrained Optimization

- Problems of the sort:

\[ \min_{x \in D} f(x) \quad \text{arg min}_{x \in D} f(x) \]
Constrained Optimization

- Problems of the sort:

\[
\min_{x \in D} f(x) \quad \arg \min_{x \in D} f(x)
\]
Constrained Optimization

- Examples:

  - minimize: \( E(v, x) = \frac{1}{2} m \| v \|_2^2 + mg^T x \)
  - subject to: \( \| x - x_0 \|_2 = L \)
Constrained Optimization

- Examples:
  - minimize: \( f(x) = c^T x \)
  - subject to: \( Ax - b \leq 0 \)
    \[
    x \geq 0
    \]
Constrained Optimization

• In general:
  • minimize: \( f(x) \)
  • subject to: \( c(x) = 0 \)
    \[ h(x) \geq 0 \]

• One approach is to approximate the problem as unconstrained – penalty methods:
  • minimize:
    \[
    F(x) = f(x) + \frac{1}{2\mu} \left( \|c(x)\|_2^2 + \sum_{i=1}^{N} H(-h_i(x))h_i(x)^2 \right)
    \]
  • as \( \mu \to 0 \)
  • with \( H(x \geq 0) = 1, H(x < 0) = 0 \)
Equality Constraints

• Method of Lagrange multipliers
  • minimize: \( f(x) \)
  • subject to: \( c(x) = 0 \)
• What are the necessary conditions for defining a minimum?
  • Taylor expansion of \( f(x) \) in some direction with \( \|d\|_2 \ll 1 \):
    \[
    f(x + d) = f(x) + g(x)^T d + \ldots
    \]
  • either \( g(x) = 0 \) or \( g(x) \perp d \) at the minimum
• For equality constraints, \( c(x) = 0 \), and \( c(x + d) = 0 \)
  • Taylor expansion of \( c(x) \) in the same direction:
    \[
    c(x + d) = c(x) + \nabla c(x) \cdot d + \ldots \Rightarrow d \perp \nabla c(x)
    \]
• Therefore, \( g(x) \parallel \nabla c(x) \Rightarrow g(x) - \lambda \nabla c(x) = 0 \)
Equality Constraints

• Example

• minimize: \( f(x_1, x_2) = x_1^2 + 10x_2^2 \)

• subject to: \( c(x_1, x_2) = x_1 - x_2 - 3 = 0 \)

• Contours of the function and the constraint
Equality Constraints

• Method of Lagrange multipliers
  • minimize: \( f(x) \)
  • subject to: \( c(x) = 0 \)

• A solution to the equality constrained problem satisfies:

\[
\begin{pmatrix}
g(x) - \lambda \nabla c(x) \\
c(x)
\end{pmatrix} = 0
\]

• For the unknowns: \( x, \lambda \)

• \( \lambda \) is called a Lagrange multiplier

• The solution set \( (x, \lambda) \) is a critical point of:

\[
L(x, \lambda) = f(x) - \lambda c(x)
\]

• called the “Lagrangian”
Equality Constraints

• Example
  
  • minimize: \( f(x_1, x_2) = x_1^2 + 10x_2^2 \)
  
  • subject to: \( c(x_1, x_2) = x_1 - x_2 - 3 = 0 \)

  • Contours of the function and the constraint
Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(x)$
  - subject to: $c(x) = 0$

- What are the necessary conditions for defining a minimum?
  - Taylor expansion of $f(x)$ in some direction with $\|d\|_2 \ll 1$:
    $$f(x + d) = f(x) + g(x)^T d + \ldots$$
  - either $g(x) = 0$ or $g(x) \perp d$ at the minimum

- For equality constraints, $c(x) = 0$, and $c(x + d) = 0$
  - Taylor expansion of $c(x)$ in the same direction:
    $$c(x + d) = c(x) + J_c(x)d + \ldots$$
  - The direction belongs to what set of vectors?
Equality Constraints

• Method of Lagrange multipliers
  • minimize: \( f(x) \)
  • subject to: \( c(x) = 0 \)

• What are the necessary conditions for defining a minimum?
  • Taylor expansion of \( f(x) \) in some direction with \( \|d\|_2 \ll 1 \):
    \[
    f(x + d) = f(x) + g(x)^T d + \ldots
    \]
  • either \( g(x) = 0 \) or \( g(x) \perp d \) at the minimum
  • If \( J_c(x)d = 0 \) and \( g(x) \perp d \),
    • then \( g(x) \) at the minimum belongs to what set of vectors?

• Therefore:
Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(x)$
  - subject to: $c(x) = 0$
- What are the necessary conditions for defining a minimum?
  - Taylor expansion of $f(x)$ in some direction with $\|d\|_2 \ll 1$:
    $$f(x + d) = f(x) + g(x)^T d + \ldots$$
  - either $g(x) = 0$ or $g(x) \perp d$
  - If $J_c(x)d = 0$ and $g(x) \perp d$,
    - then $g(x)$ at the minimum belongs to what set of vectors?
- Therefore:
Equality Constraints

- Method of Lagrange multipliers
  - minimize: $f(x)$
  - subject to: $c(x) = 0$

- A solution to the equality constrained problem satisfies:
  \[
  \begin{pmatrix}
  g(x) - J_c(x)^T \lambda \\
  c(x)
  \end{pmatrix} = 0
  \]

- For the unknowns: $x, \lambda$
- $\lambda$ is a vector of Lagrange multiplier
- The solution set $(x, \lambda)$ is a critical point of:
  \[ L(x, \lambda) = f(x) - c(x)^T \lambda \]
  - called the “Lagrangian”
Inequality Constraints

- Interior point methods
  - minimize: $f(x)$
  - subject to: $h(x) \geq 0$
- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $f(x) - \mu \sum_{i=1}^{N} \log(h_i(x))$
  - as $\mu \to 0^+$
- For $h_i(x) \to 0$, the objective function becomes large
  - This creates a barrier from which an unconstrained optimization scheme may not escape.
- Determining the minimum of this new objective function for progressively weaker barriers ($\mu \to 0^+$) is important.
- How can this be done reliably?
Inequality Constraints

- Interior point methods, example
  - minimize: $x$
  - subject to: $x \geq 0$
- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $x - \mu \log(x)$
Inequality Constraints

- Interior point methods:
  - minimize: \( f(x) \)
  - subject to: \( h(x) \geq 0 \)

- Rewrite as unconstrained optimization by using a barrier:
  - minimize: \( f(x) - \mu \sum_{i=1}^{N} \log(h_i(x)) \)
  - as \( \mu \to 0^+ \)

- Why a logarithmic barrier?

- The minimum of the unconstrained problem is found where:
Inequality Constraints

- Interior point methods:
  - minimize: $f(x)$
  - subject to: $h(x) \geq 0$

- Rewrite as unconstrained optimization by using a barrier:
  - minimize: $f(x) - \mu \sum_{i=1}^{N} \log(h_i(x))$
  - as $\mu \rightarrow 0^+$

- Use __________ to study a sequence of barrier parameters

- Stop __________ when:
Inequality Constraints

• Example:

• minimize: $f(x_1, x_2) = x_1^2 + 10x_2^2$

• subject to: $h(x_1, x_2) = 1 - (x_1 - 2)^2 - (x_2 - 2)^2 \geq 0$

• Contours of the function and the constraint
Inequality Constraints

\[ f = @(x) x(1)^2 + 10 \times x(2)^2; \]
\[ \text{grad}_f = @(x) \begin{bmatrix} 2x(1); 20x(2) \end{bmatrix}; \]
\[ H_f = @(x) \begin{bmatrix} 2 & 0; 0 & 20 \end{bmatrix}; \]

\[ h = @(x) 1 - (x(1) - 2)^2 - (x(2) - 2)^2; \]
\[ \text{grad}_h = @(x) \begin{bmatrix} -2(x(1)-2); -2(x(2)-2) \end{bmatrix}; \]
\[ H_h = @(x) \begin{bmatrix} -2 & 0; 0 & -2 \end{bmatrix}; \]

\[ \phi = @(x,\mu) f(x) - \mu \times \log(h(x)); \]
\[ \text{grad}_{\phi} = @(x,\mu) \text{grad}_f(x) - \mu / h(x) \times \text{grad}_h(x); \]
\[ H_{\phi} = @(x,\mu) H_f(x) - \mu / h(x) \times H_h(x) + \mu / h(x)^2 \times \text{grad}_h(x) \times \text{grad}_h(x)'; \]

\[ x = \begin{bmatrix} 2; 2 \end{bmatrix}; \]

for \( \mu = [1:-0.01:0.01] \)

\[ \text{while ( norm( \text{grad}_{\phi}(x, \mu) ) > 1e-8 )} \]

\[ x = x - H_{\phi}(x, \mu) \backslash \text{grad}_{\phi}(x, \mu); \]

end;

end;
Inequality Constraints

• Example:

  • minimize: \( f(x_1, x_2) = x_1^2 + 10x_2^2 \)
  
  • subject to: \( h(x_1, x_2) = 1 - (x_1 - 2)^2 - (x_2 - 2)^2 \geq 0 \)

• Contours of the function and the constraint
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