Unconstrained Minimization (I)

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Outline

- Unconstrained Minimization Problems
  - Basic Terminology
  - Examples
  - Strong Convexity
  - Smoothness
- Descent Methods
  - General Descent Method
  - Exact Line Search
  - Backtracking Line Search

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Basic Terminology

□ Unconstrained Optimization Problem

$$\min\ f(x)$$

- $f(x): \mathbf{R}^n \rightarrow \mathbf{R}$ is convex
- $f(x)$ always have a domain $\mathrm{dom}\, f$
  - ✓ $\mathrm{dom}\, f = \mathbf{R}^n$, $\mathrm{dom}\, f \subset \mathbf{R}^n$
- $f(x)$ is twice continuously differentiable
  - ✓ $\mathrm{dom}\, f$ is open, such as $(0, \infty)$
- The problem is solvable
  - ✓ There exists an optimal point x^*

$$\inf_x f(x) = f(x^*) = p^*$$

Basic Terminology

Unconstrained Optimization Problem

$$\min \; f(x)$$

- x^* is optimal if and only if — Equivalent

$$\nabla f(x^*) = 0$$

- Special cases: a closed-form solution
- General cases: an iterative algorithm
  - ✓ A sequence of points $x^{(0)}, x^{(1)}, \ldots \in \mathbf{dom}\, f$ with
    $$f\left(x^{(k)}\right) \to p^* \text{ as } k \to \infty$$
  - ✓ A minimizing sequence for the problem
  - ✓ The algorithm is terminated when
    $$f\left(x^{(k)}\right) - p^* \;\leq \epsilon$$

Requirements of Iterative Algorithm

- Initial Point
  - A suitable starting point

$$x^{(0)} \in \operatorname{dom} f$$

- Sublevel Set is Closed

$$S = \{x \in \operatorname{dom} f \mid f(x) \le f(x^{(0)})\}$$

  - Satisfied for all $x^{(0)} \in \operatorname{dom} f$ if the function f is closed
    - ✓ Continuous functions with $\operatorname{dom} f = \mathbf{R}^n$
    - ✓ Continuous functions with open domains and $f(x) \to \infty$ as $x \to \operatorname{bd} \operatorname{dom} f$

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Examples

- Convex Quadratic Minimization Problem

$$\min \quad \frac{1}{2}x^\top P x + q^\top x + r$$

  - $P \in \mathbf{S}_+^n, q \in \mathbf{R}^n, r \in \mathbf{R}$
  - Optimality Condition

$$Px^* + q = 0$$

1. $P \succ 0 \Rightarrow x^* = -P^{-1}q$ (unique solution)
2. If P is singular and $q \in \mathcal{R}(P)$, any solution of $Px^* + q = 0$ is optimal
3. If $q \notin \mathcal{R}(P)$, no solution, unbound below

Examples

- Convex Quadratic Minimization Problem

$$\min \quad \frac{1}{2}x^\top Px + q^\top x + r$$

  - $P \in \mathbf{S}_+^n, q \in \mathbf{R}^n, r \in \mathbf{R}$

3. If $q \notin \mathcal{R}(P)$, no solution, unbound below
   - ✓ $q = a + b$, $a \in \mathcal{R}(P)$, $b \perp \mathcal{R}(P)$, $a \perp b$
   - ✓ Let $x = tb$

$$\begin{aligned} &\frac{1}{2}x^\top Px + q^\top x + r \\ &= t(a+b)^\top b + r \\ &= t\|b\|_2^2 + r \end{aligned}$$

Examples

Least-Squares Problem

$$\min \quad \|Ax - b\|_2^2 = x^\top A^\top Ax - 2b^\top Ax + b^\top b$$

- $A \in \mathbf{R}^{m\times n}, b \in \mathbf{R}^m$ are problem data

- Optimality Condition

$$\nabla f(x^*) = 2A^\top Ax^* - 2A^\top b = 0$$

- Normal Equations

$$A^\top Ax^* = A^\top b$$

Examples

- ☐ Unconstrained Geometric Programming

$$\min \quad f(x) = \log\left(\sum_{i=1}^{m} \exp\left(a_i^\top x + b_i\right)\right)$$

  - Optimality Condition

$$\nabla f(x^*) = \frac{\sum_{i=1}^{m} \exp\left(a_i^\top x^* + b_i\right) a_i}{\sum_{i=1}^{m} \exp\left(a_i^\top x^* + b_i\right)} = 0$$

    - ✓ No analytical solution
  - An Iterative Algorithm
    - ✓ $\operatorname{dom} f = \mathbf{R}^n$, any point can be chosen as $x^{(0)}$

Examples

Analytic Center of Linear Inequalities

$$\min \quad f(x) = -\sum_{i=1}^{m} \log(b_i - a_i^\top x)$$

- $\operatorname{dom} f = \{x \mid a_i^\top x < b_i, i = 1,2,\ldots,m\}$
- f is called as the logarithmic barrier for the inequalities $a_i^\top x < b_i$
- The solution of this problem is called the analytic center of the inequalities
- An Iterative Algorithm
  - ✓ $x^{(0)}$ must satisfy $a_i^\top x^{(0)} < b_i$

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Strong Convexity

- $f(\cdot)$ is strongly convex on S, if $\exists\, m > 0$

$$\nabla^2 f(x) \succcurlyeq mI, \qquad \forall x \in S$$

1. A Quadratic Lower Bound

- $\forall x, y \in S, \exists z \in [x, y]$

$$f(y) = f(x) + \nabla f(x)^\top (y-x) + \frac{1}{2}(y-x)^\top \nabla^2 f(z)(y-x)$$

$$\geq f(x) + \nabla f(x)^\top (y-x) + \frac{m}{2}\|y-x\|_2^2$$

Strong Convexity

- $f(\cdot)$ is strongly convex on S, if $\exists\, m > 0$

$$\nabla^2 f(x) \succcurlyeq mI, \qquad \forall x \in S$$

1. A Quadratic Lower Bound

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) + \frac{m}{2}\|y - x\|_2^2, \qquad \forall x, y \in S$$

- When $m = 0$, reduce to the first-order condition of convex functions

Strong Convexity

- $f(\cdot)$ is strongly convex on S, if $\exists\, m > 0$

$$\nabla^2 f(x) \succcurlyeq mI, \qquad \forall x \in S$$

1. A Quadratic Lower Bound

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) + \frac{m}{2} \|y - x\|_2^2, \qquad \forall x, y \in S$$

2. A Condition for Suboptimality

$$\begin{aligned} f(y) &\geq \min_y f(x) + \nabla f(x)^\top (y - x) + \frac{m}{2} \|y - x\|_2^2 \\ &= f(x) + \nabla f(x)^\top (\tilde{y} - x) + \frac{m}{2} \|\tilde{y} - x\|_2^2, \;\; \tilde{y} = x - \frac{1}{m} \nabla f(x) \\ &= f(x) - \frac{1}{2m} \|\nabla f(x)\|_2^2 \end{aligned}$$

Strong Convexity

- $f(\cdot)$ is strongly convex on S, if $\exists\, m > 0$

$$\nabla^2 f(x) \succcurlyeq mI, \qquad \forall x \in S$$

1. A Quadratic Lower Bound

$$f(y) \geq f(x) + \nabla f(x)^{\top}(y - x) + \frac{m}{2}\|y - x\|_2^2, \qquad \forall x, y \in S$$

2. A Condition for Suboptimality

$$p_* \geq f(x) - \frac{1}{2m}\|\nabla f(x)\|_2^2 \Rightarrow f(x) - p_* \leq \frac{1}{2m}\|\nabla f(x)\|_2^2$$

- If the gradient is small at x, then it is nearly optimal

$$\|\nabla f(x)\|_2 \leq (2m\epsilon)^{\frac{1}{2}} \Rightarrow f(x) - p^* \leq \epsilon$$

Strong Convexity

- $f(\cdot)$ is strongly convex on S, if $\exists\, m > 0$

$$\nabla^2 f(x) \succcurlyeq mI, \qquad \forall x \in S$$

3. An Upper Bound of $\|x^* - x\|_2$

$$\begin{aligned}
p_* &= f(x^*) \\
&\geq f(x) + \nabla f(x)^{\mathsf{T}}(x^* - x) + \frac{m}{2}\|x^* - x\|_2^2 \\
&\geq f(x) - \|\nabla f(x)\|_2 \|x^* - x\|_2 + \frac{m}{2}\|x^* - x\|_2^2 \\
&\geq p_* - \|\nabla f(x)\|_2 \|x^* - x\|_2 + \frac{m}{2}\|x^* - x\|_2^2
\end{aligned}$$

Strong Convexity

- $f(\cdot)$ is strongly convex on S, if $\exists\, m > 0$

$$\nabla^2 f(x) \succcurlyeq mI, \qquad \forall x \in S$$

3. An Upper Bound of $\|x^* - x\|_2$

$$\frac{m}{2}\|x^* - x\|_2^2 \le \|\nabla f(x)\|_2 \|x^* - x\|_2$$

$$\Longrightarrow \quad \|x^* - x\|_2 \le \frac{2}{m}\|\nabla f(x)\|_2$$

- $x \to x^*$, as $\nabla f(x) \to 0$
- The optimal point x^* is unique

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Smoothness

- $f(\cdot)$ is smooth on S, if $\exists\, M > 0$

$$\nabla^2 f(x) \preccurlyeq MI, \qquad \forall x \in S$$

1. A Quadratic Upper Bound

- $\forall x, y \in S, \exists z \in [x, y]$

$$f(y) = f(x) + \nabla f(x)^\top (y - x) + \frac{1}{2}(y - x)^\top \nabla^2 f(z)(y - x)$$

$$\leq f(x) + \nabla f(x)^\top (y - x) + \frac{M}{2}\|y - x\|_2^2$$

Smoothness

- $f(\cdot)$ is smooth on S, if $\exists\, M > 0$

$$\nabla^2 f(x) \preccurlyeq MI, \qquad \forall x \in S$$

1. A Quadratic Upper Bound

$$f(y) \leq f(x) + \nabla f(x)^\top (y - x) + \frac{M}{2}\|y - x\|_2^2, \qquad \forall x, y \in S$$

2. An Upper Bound of Gradients

$$\min_y f(y) \leq \min_y f(x) + \nabla f(x)^\top (y - x) + \frac{M}{2}\|y - x\|_2^2$$

$$= f(x) + \nabla f(x)^\top (\tilde{y} - x) + \frac{M}{2}\|\tilde{y} - x\|_2^2, \ \tilde{y} = x - \frac{1}{M}\nabla f(x)$$

$$= f(x) - \frac{1}{2M}\|\nabla f(x)\|_2^2$$

Smoothness

- $f(\cdot)$ is smooth on S, if $\exists\, M > 0$

$$\nabla^2 f(x) \preccurlyeq MI, \qquad \forall x \in S$$

1. A Quadratic Upper Bound

$$f(y) \leq f(x) + \nabla f(x)^\top (y - x) + \frac{M}{2}\|y - x\|_2^2, \qquad \forall x, y \in S$$

2. An Upper Bound of Gradients

$$p^* \leq f(x) - \frac{1}{2M}\|\nabla f(x)\|_2^2$$

$$\Rightarrow \quad \frac{1}{2M}\|\nabla f(x)\|_2^2 \leq f(x) - p_*$$

Condition Number

- Condition Number of a Matrix A

$$\mathrm{cond}(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$$

- $f(\cdot)$ is both strongly convex and smooth

$$mI \preccurlyeq \nabla^2 f(x) \preccurlyeq MI, \qquad \forall x \in S$$

  - Condition number of f

$$\kappa = \frac{M}{m} \geq \mathrm{cond}\left(\nabla^2 f(x)\right)$$

  - Has a strong effect on the efficiency of optimization methods

Condition Number

Geometric Interpretations

- Width of a convex set $C \subseteq \mathbf{R}^n$, in the direction q where $\|q\|_2 = 1$

$$W(C,q) = \sup_{z \in C} q^\top z - \inf_{z \in C} q^\top z$$

- Minimum width and maximum width of C

$$W_{\min} = \inf_{\|q\|_2=1} W(C,q), \qquad W_{\max} = \sup_{\|q\|_2=1} W(C,q)$$

- Condition number of C
  - ✓ $\mathrm{cond}(C)$ is small implies C it is nearly spherical

$$\mathrm{cond}(C) = \frac{W_{\max}^2}{W_{\min}^2}$$

Condition Number

Geometric Interpretations

- α-sublevel set of f

$$C_\alpha = \{x | f(x) \le \alpha\}, \qquad p^* \le \alpha \le f(x_0)$$

- $f(\cdot)$ is both strongly convex and smooth

$$p_* + \frac{M}{2}\|y - x^*\|_2^2 \ge f(y) \ge p_* + \frac{m}{2}\|y - x^*\|_2^2$$

$$B_{\text{inner}} \subseteq C_\alpha \subseteq B_{\text{outer}}$$

$$B_{\text{inner}} = \left\{ y \,\middle|\, \|y - x^*\| \le \left(\frac{2(\alpha - p^*)}{M}\right)^{1/2} \right\} \qquad B_{\text{outer}} = \left\{ y \,\middle|\, \|y - x^*\| \le \left(\frac{2(\alpha - p^*)}{m}\right)^{1/2} \right\}$$

Condition Number

Geometric Interpretations

- α-sublevel set of f

$$C_\alpha = \{x | f(x) \leq \alpha\}, \qquad p^* \leq \alpha \leq f(x_0)$$

- $f(\cdot)$ is both strongly convex and smooth

$$p_* + \frac{M}{2}\|y - x^*\|_2^2 \geq f(y) \geq p_* + \frac{m}{2}\|y - x^*\|_2^2$$

$$y \in C_\alpha \Rightarrow a \geq f(y) \Rightarrow a \geq p_* + \frac{m}{2}\|y - x^*\|_2^2$$

$$\Rightarrow \frac{m}{2}\|y - x^*\|_2^2 \leq a - p_* \quad \Rightarrow \|y - x^*\| \leq \sqrt{\frac{2}{m}(a - p_*)}$$

$$\Rightarrow y \in B_{\text{outer}} = \left\{ y \,\middle|\, \|y - x^*\| \leq \left(\frac{2(\alpha - p^*)}{m}\right)^{1/2} \right\} \Rightarrow C_\alpha \subseteq B_{\text{outer}}$$

Condition Number

Geometric Interpretations

- α-sublevel set of f

$$C_\alpha = \{x | f(x) \leq \alpha\}, \qquad p^* \leq \alpha \leq f(x_0)$$

- $f(\cdot)$ is both strongly convex and smooth

$$p_* + \frac{M}{2}\|y - x^*\|_2^2 \geq f(y) \geq p_* + \frac{m}{2}\|y - x^*\|_2^2$$

$$y \in B_{\text{inner}} = \left\{ y \,\middle|\, \|y - x^*\| \leq \left(\frac{2(\alpha - p^*)}{M}\right)^{1/2} \right\}$$

$$\Rightarrow f(y) \leq p_* + \frac{M}{2}\|y - x^*\|_2^2 \leq \alpha \Rightarrow y \in C_\alpha \Rightarrow B_{\text{inner}} \subseteq C_\alpha$$

Condition Number

- Geometric Interpretations
  - α-sublevel set of f

$$C_\alpha = \{x | f(x) \le \alpha\}, \qquad p^* \le \alpha \le f(x_0)$$

  - $f(\cdot)$ is both strongly convex and smooth

$$B_{\text{inner}} \subseteq C_\alpha \subseteq B_{\text{outer}}$$

$$B_{\text{inner}} = \left\{ y \,\middle|\, \|y - x^*\| \le \left(\frac{2(\alpha - p^*)}{M} \right)^{1/2} \right\} \quad B_{\text{outer}} = \left\{ y \,\middle|\, \|y - x^*\| \le \left(\frac{2(\alpha - p^*)}{m} \right)^{1/2} \right\}$$

  - Condition number of C_α

$$\text{cond}(C_\alpha) \le \kappa = \frac{M}{m}$$

Discussions

- Parameters m and M
  - Known only in rare cases
  - Unknown in general
- They are conceptually useful
  - They establish that the algorithm converges
  - The convergence behavior of optimization algorithms depends on them
- In Practice
  - Estimate their values
  - Design parameter-free algorithms

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Iterative Methods

- A Minimizing Sequence

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}, \qquad k = 1, \ldots$$

  - k is the the iteration number
  - $x^{(k)}$ is the output of iterative methods
  - $\Delta x^{(k)}$ is the step or search direction
  - $t^{(k)} \geq 0$ is the step size or step length

- Shorthand

$$x := x + t\Delta x$$

Descent Methods

□ Descent Methods

$$f\left(x^{k+1}\right) < f\left(x^{k}\right)$$

- Except when $x^{(k)}$ is optimal
- $\forall k,\ x^{(k)} \in S = \{x \in \mathrm{dom}\, f \mid f(x) \le f(x^{(0)})\}$
- The search direction makes an acute angle with the negative gradient

$$\nabla f\left(x^{(k)}\right)^{\top} \Delta x^{(k)} < 0$$

$$\left.\begin{array}{r} f\left(x^{k+1}\right) \ge f\left(x^{k}\right) + \nabla f\left(x^{(k)}\right)^{\top}(x^{k+1} - x^{k}) \\ \nabla f\left(x^{(k)}\right)^{\top} \Delta x^{(k)} \ge 0 \Rightarrow \nabla f\left(x^{(k)}\right)^{\top}\left(x^{k+1} - x^{k}\right) \ge 0 \end{array}\right\} \Rightarrow f\left(x^{k+1}\right) \ge f\left(x^{k}\right)$$

Descent Methods

☐ Descent Methods

$$f\left(x^{k+1}\right) < f\left(x^{k}\right)$$

- Except when $x^{(k)}$ is optimal
- $\forall k,\ x^{(k)} \in S = \{x \in \mathrm{dom}\, f \mid f(x) \leq f(x^{(0)})\}$
- The search direction makes an acute angle with the negative gradient

$$\nabla f\left(x^{(k)}\right)^{\top} \Delta x^{(k)} < 0$$

- $\Delta x^{(k)}$ is called as descent direction

General Descent Method

The Algorithm

Given a starting point $x \in \mathrm{dom}\, f$

Repeat

1. Determine a descent direction Δx.
2. Line search: Choose a step size $t \geq 0$.
3. Update: $x := x + t\Delta x$.

until stopping criterion is satisfied.

Line Search

- Determine the next iterate along the line

$$\{x + t\Delta x | t \in \mathbf{R}_+\}$$

General Descent Method

The Algorithm

Given a starting point $x \in \mathrm{dom}\, f$

Repeat

1. Determine a descent direction Δx.
2. Line search: Choose a step size $t \geq 0$.
3. Update: $x := x + t\Delta x$.

until stopping criterion is satisfied.

Stopping Criterion

$$\|\nabla f(x)\|_2 \leq \eta$$

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Exact Line Search

- Minimize f along the Ray

$$t = \mathrm{argmin}_{s \geq 0} f(x + s\Delta x)$$

  - The cost of the minimization problem with one variable is low

$$\min_{s \geq 0} f(x + s\Delta x)$$

  - The minimizer along the ray can be found analytically

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Backtracking Line Search

- Most line searches used in practice are inexact
  - Approximately minimize f along the ray
  - Just reduce f 'enough'

- Backtracking Line Search

  given a descent direction Δx for f at $x \in$ **dom** f, $\alpha \in (0, 0.5)$, $\beta \in (0, 1)$

  $t := 1$

  while $f(x + t\Delta x) > f(x) + \alpha t \nabla f(x)^\top \Delta x$, $t := \beta t$

Backtracking Line Search

- The line search is called backtracking
  - It starts with unit step size and then reduces it by the factor β

$$t := 1, \qquad t := \beta t$$

- It eventually terminates
  - Δx is a descent direction, i.e., $\nabla f(x)^\top \Delta x < 0$
  - For small enough t

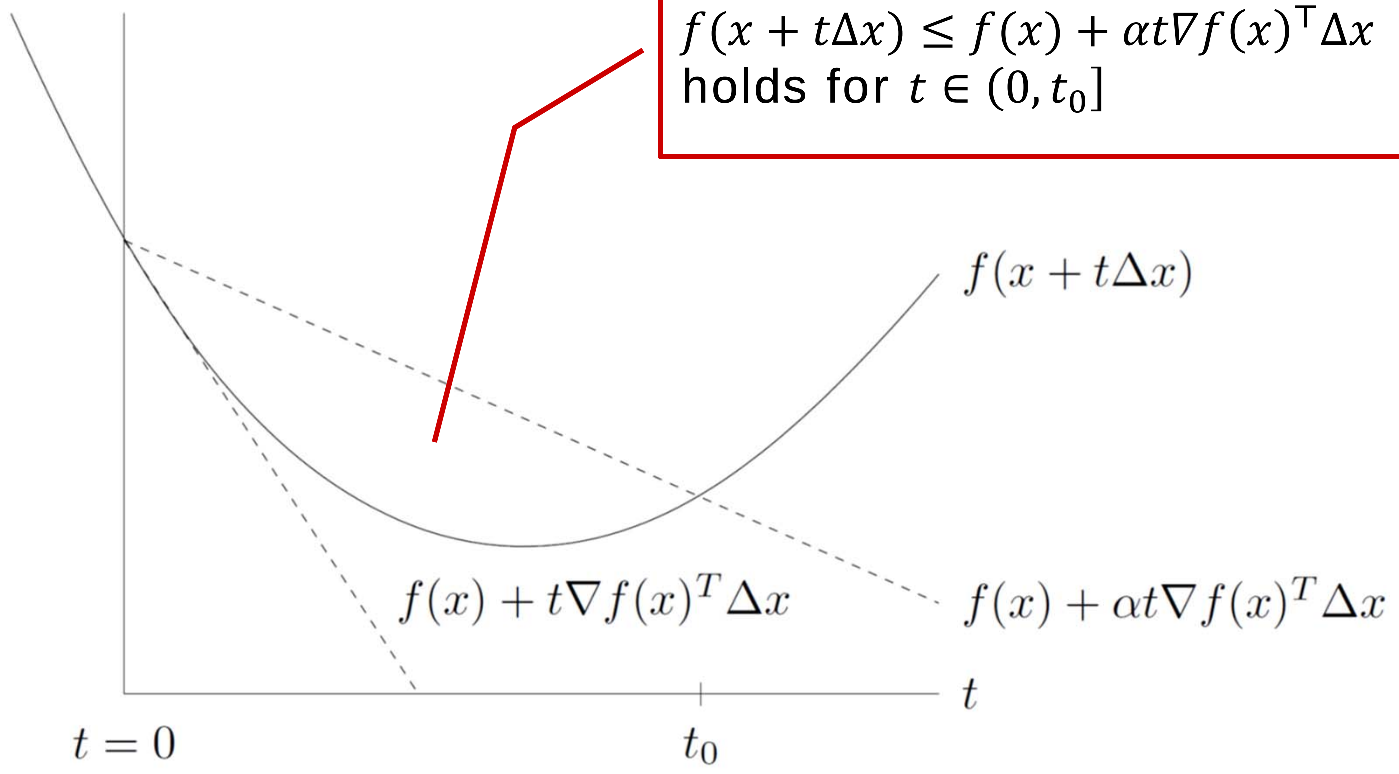
$$f(x + t\Delta x) \approx f(x) + t\nabla f(x)^\top \Delta x < f(x) + \alpha t \nabla f(x)^\top \Delta x$$

  - ✓ α is the fraction of the decrease in f predicted by linear extrapolation that we will accept

Backtracking Line Search

Graph Interpretation

The backtracking exit inequality $f(x+t\Delta x) \le f(x) + \alpha t \nabla f(x)^{\mathrm{T}} \Delta x$ holds for $t \in (0, t_0]$

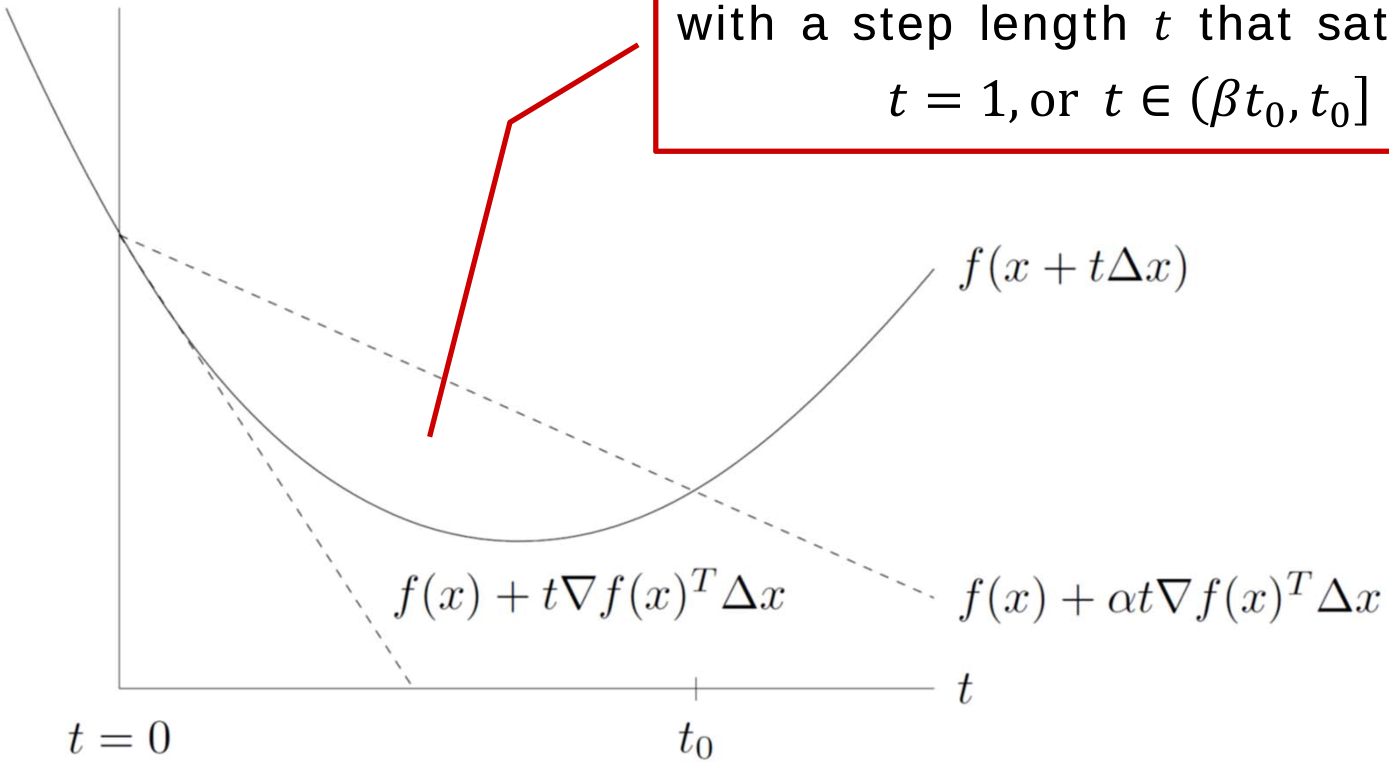


Backtracking Line Search

Graph Interpretation

The backtracking line search stops with a step length t that satisfies

$$t = 1, \text{or } t \in (\beta t_0, t_0]$$

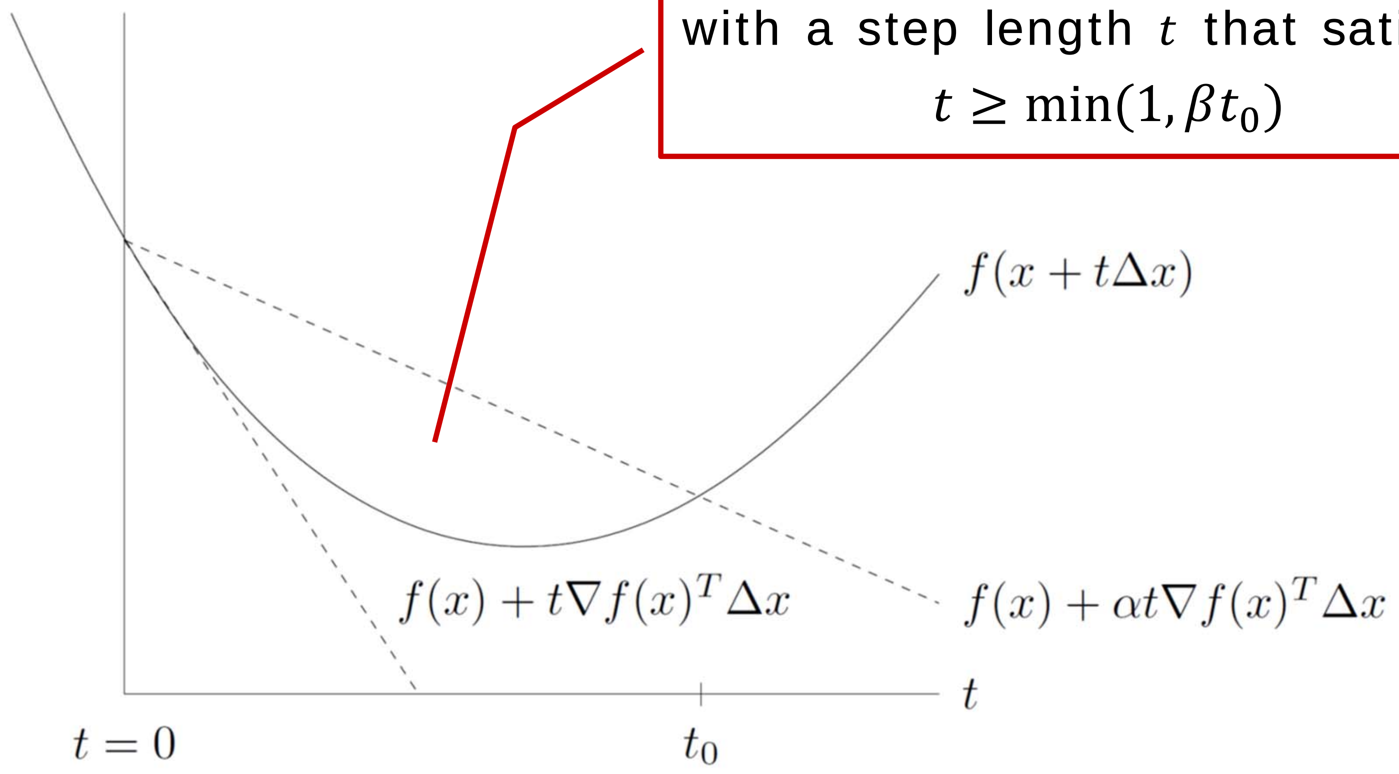


Backtracking Line Search

□ Graph Interpretation

The backtracking line search stops with a step length t that satisfies

$$t \geq \min(1, \beta t_0)$$



Backtracking Line Search

- $\mathbf{dom}\, f \neq \mathbf{R}^n$

$$f(x + t\Delta x) \leq f(x) + \alpha \nabla f(x)^\top \Delta x$$

  - Require $x + t\Delta x \in \mathbf{dom}\, f$

- A Practical Implementation
  1. Multiply t by β until $x + t\Delta x \in \mathbf{dom}\, f$
  2. Check whether the above inequality holds
  - α is typically chosen between 0.01 and 0.3
  - β is often chosen between 0.1 and 0.8

Summary

- Unconstrained Minimization Problems
  - First-order Optimality Condition
  - Strong Convexity and Implications
  - Smoothness and Implications

- Descent Methods
  - General Descent Method
  - Exact Line Search
  - Backtracking Line Search