Math 6880/7875: Advanced Optimization
Background and Review: Optimization

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Several topics are background for this course:

- (Numerical) linear algebra
- Probability/statistics
- “Basic” optimization knowledge

We’ll spend some time briefly reviewing portions of these.
Optimization

General optimization problem:

\[
\begin{align*}
\text{minimize} & \quad f(x) \\
\text{subject to} & \quad x \in S \\
S & := \{ x \mid g_i(x) \leq 0, \ i \in [m] \}
\end{align*}
\]

- \( x = (x_1, \ldots, x_n)^T \in \mathbb{R}^n \) is the optimization or design variable
- \( f : \mathbb{R}^n \to \mathbb{R} \) is the objective function
- \( g_i : \mathbb{R}^n \to \mathbb{R}, \ i \in [m] \), are the constraints
- \( S \) is the feasible set

We will always consider \( n < \infty \), but we will occasionally allow \( m \uparrow \infty \)

- If \( m > 0 \), the problem is constrained; otherwise it is unconstrained
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- We will always consider \( n < \infty \), but we will occasionally allow \( m \uparrow \infty \)
- If \( m > 0 \), the problem is \textbf{constrained}; otherwise it is \textbf{unconstrained}

(implicitly \( S = \mathbb{R}^n \))
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Solutions to optimization problems have their own taxonomy and properties:

- A point \( x \in \mathbb{R}^n \) is \textbf{feasible} if \( x \in S \).
- A point \( x^* \in \mathbb{R}^n \) is a ("global") \textbf{solution}, \textbf{optimum}, or \textbf{optimal point} if \( f(x^*) \leq f(x) \) for every \( x \in S \).
- A point \( x^* \in \mathbb{R}^n \) is a "local" solution, optimum, or optimal point if \( \exists \epsilon > 0 \) such that \( f(x^*) \leq f(x) \) for all \( x \in B_\epsilon(x^*) \cap S \), where

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Solutions to optimization problems have their own taxonomy and properties:
- “Optimum”/“extremum” $\leftrightarrow$ “maximum”/“minimum”, as appropriate
- Maximization of $f$ is minimization of $-f$
- Optimization problems can have zero, one, or many solutions. Which of these is true is rarely obvious.

Generally our goal is to find/compute an optimal solution. A local one could suffice.

- equality constraints are doable: $h(x) = 0$
  \[
  g_i(x) = h(x) \\
g_2(x) = -h(x)
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Optimization

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Simple examples

Example
One, unique solution

\[
\min_{x \in \mathbb{R}} |x|
\]
subject to \( x \geq -1 \)

Example
No solutions – infeasible

\[
\min_{x \in \mathbb{R}} x^2
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subject to \( |x| \leq -1 \)
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**Example**
No solutions – unbounded

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\max_{x \in \mathbb{R}} x^2
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**Example**
Many solutions

\[
\min_{x \in \mathbb{R}} \sin x
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subject to \(|x| \geq \pi\)
Simple examples

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\[ \max_{x \in \mathbb{R}} x^2 \]

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Ascertaining optimality

In some special cases, with some effort, one can conclude global optimality.

- **Direct methods** – Analytically prove global optimality. (E.g.,
  \[ f(x) = (x^2 - 1)^{10} \]

- **Quadratic functions** – \( f \) is quadratic with a positive-definite Hessian.

  - **Coercive functions** – Global optimality in some ball \( B \), and show that that \( f \) outside \( B \) dominates \( f \) inside \( B \).
  
  - **Globally convex functions** – Ensures that local minima are global minima.

Caveats:

- All the above are “easier” for unconstrained optimization, and become much more technical and difficult for constrained optimization.

- *Global* optimality requires some *global* knowledge of the objective and constraints.

- In high dimensions (\( n \) large), globally certifying any property of generic functions is hard.

The depressing fact of life: without relatively strong assumptions, local optimality is the best we know how to establish.
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Local optimality

There are a handful of **optimality conditions** that can be sufficient and/or necessary to determine local optimality.

- First-order optimality conditions – conditions involving the gradients of $f$ and/or $g_i$.
- Second-order optimality conditions – conditions involving Hessians. Less computationally useful due to complexity/storage requirements.

It’s much easier to discuss these conditions for unconstrained optimization first.
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First-order local optimality: unconstrained optimization

**Unconstrained optimization:**

\[
\text{minimize } f(x),
\]

which implicitly allows \( x \in \mathbb{R}^n \). (i.e., the feasible set is \( S = \mathbb{R}^n \).)

The simplest first-order local optimality condition is a necessary one.

**Theorem**

If \( f \in C^1(\mathbb{R}^n) \), then \( x^* \) is a local minimum only if \( \nabla f(x^*) = 0 \).

**Proof.**

Fix \( i \in [n] \). Let \( x_i \) be free, but fix \( x_{\setminus i} = x_{\setminus i}^* \).

The resulting one-dimensional function \( f_i \) must have a local minimum at \( x_i = x_i^* \), where its univariate derivative vanishes.

Repeat for every \( i \implies \nabla f(x^*) = 0 \).

**Notes:**

- \( \nabla f(x^*) = 0 \) is not sufficient to conclude anything.
- \( \nabla f(x^*) = 0 \) is also a necessary condition for local minimization over \( S \subset \mathbb{R}^n \) so long as \( x^* \in \text{int}(S) \).
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Stationary points and definite matrices

Given $f : \mathbb{R}^n \to \mathbb{R}$ that is differentiable, a point $x$ satisfying $\nabla f(x) = 0$ is a stationary point.

- Stationary points can be local/global minima.
- Stationary points can be local/global maxima.
- Stationary points can be saddle points (neither a maximum nor a minimum).

Many computational methods attempt to compute stationary points, even if we can’t classify the result.

Stationary points are not necessarily easy to compute....
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Definite matrices

Quadratic classification of matrices are needed for second-order conditions:

- A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is **positive definite** if $x^T A x > 0$ for every $x \in \mathbb{R}^n \setminus \{0\}$.
  
  We write $A > 0$.
  
  (Equivalently, the inequality holds for all $x$ with unit norm.)

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- Similar definitions for negative definite, and negative semi-definite. ($A < 0$, $A \leq 0$, respectively)

- Matrices that are not positive/negative definite are **indefinite**.

We will, in particular, utilize these characterizations for Hessian matrices, $\nabla^2 f$. 
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Second-order local optimality: unconstrained optimization

**Unconstrained optimization:**

\[
\minimize f(x),
\]

An initial, necessary second-order condition:

**Theorem**

Assume \( f \in C^2(\mathbb{R}^n) \). If \( x^* \) is a local minimum, then \( \nabla^2 f(x^*) \succeq 0 \).

**Proof sketch.**

Take second-order Taylor expansion of \( f \) around \( x^* \),

\[
f(x) \approx f(x^*) + \nabla f(x^*)^T (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla^2 f(x^*) (x - x^*).\]

\( x^* \) must be a stationary point for \( f \), and the above holds for all \( x \) sufficiently close to \( x^* \).

As before, this necessary condition holds if \( x^* \) is in the interior of a feasible set for a constrained optimization problem.

\[
f(x) = x_1^2, \quad x^* = 0, \quad f''(x^*) = 0 \quad \not\Rightarrow \quad x^* \text{ is a local min}
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**Sufficient second-order optimality**

**Unconstrained optimization:**

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**Theorem**

Assume \( f \in C^2(\mathbb{R}^n) \). If \( x^* \) is a stationary point for \( f \) and \( \nabla^2 f(x^*) > 0 \), then \( x^* \) is a local minimum.

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Another second-order Taylor expansion of \( f \) for \( x \) close to \( x^* \):

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Optimality for constrained optimization

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One major complication with constrained vs. unconstrained optimization: local optima on the boundary of the feasible set must be handled with care.

Given a local optimum \( x^* \), we divide \([m]\) into active and inactive constraint sets:

- \( A(x^*) = \{ i \in [m] \mid g_i(x) = 0 \} \)
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No feasible descent: at a local minimum \( x^* \), we cannot find a direction for travel that simultaneously decreases \( f \) and all element of \( g_{A(x^*)} \).
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Constraint qualification

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To state (useful versions of) first-order optimality, we require an additional concept.

A local minimum \( x^* \) satisfies the linear independence constraint qualification (LICQ) condition if

\[\{ \nabla g_i(x^*) \}_{i \in A(x^*)},\]

is a collection of linearly independent vectors.

The LICQ condition is used to strengthen necessary local optimality conditions.
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Constrained optimization: first-order optimality

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Theorem (Karush-Kuhn-Tucker)

Assume both \( f \) and \( g_i \) are \( C^1(S) \) for every \( i \in [m] \). Assume \( x^* \) is a local minimum of the above optimization problem that satisfies the LICQ condition. Then there exists a \( \lambda \in \mathbb{R}^m \) such that \( (x^*, \lambda) \) satisfies,

\[
\begin{align*}
\nabla f(x^*) + \sum_{i \in [m]} \lambda_i \nabla g_i(x^*) &= 0 & \text{(Stationarity)} \\
\lambda_i g_i(x^*) &= 0, \ i \in [m] & \text{(Complementary Slackness)} \\
g_i(x^*) &\leq 0, \ i \in [m] & \text{(Primal feasibility)} \\
\lambda_i &\geq 0, \ i \in [m] & \text{(Dual feasibility)}
\end{align*}
\]

The above are called the **KKT conditions**, and any point \( (x, \lambda) \) satisfying these conditions (even if \( x \) is not a local minimum) is a **KKT point**.
Equality constraint (1):

\[ h(x) = 0 \Rightarrow g_1(x) = h \]
\[ g_2(x) = -h \]
\[ g_1(x) \leq 0 \]
\[ g_2(x) \leq 0 \]
\[ \Rightarrow h(x) = 0 \]

\[ \downarrow \]

\[ g_1(x) = 0 \]
\[ g_2(x) = 0 \]
KKT conditions proof idea

One proof of the KKT conditions is a combination of three ideas/techniques:

- **No feasible descent**: We cannot find any direction $d \in \mathbb{R}^n$ such that all the following hold:

\[
\nabla f(x^*)^T d < 0 \\
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- **Theorems of the alternative**: If there does not exist a $d$ satisfying the above, then there must exist a $\lambda \in \mathbb{R}^{m+1}$ with positive components satisfying

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\lambda_0 \nabla f(x^*) + \sum_{i \in \mathcal{A}(x^*)} \lambda_i \nabla g_i(x^*) = 0, \quad \lambda_i = 0, \quad i \in \mathcal{I}(x^*)
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In particular, the above exercises *Gordan’s Theorem of the alternative*.

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One proof of the KKT conditions is a combination of three ideas/techniques:

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A. Narayan  (U. Utah – Math/SCI)
KKT conditions

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\[S := \{ x \mid g_i(x) \leq 0, \ i \in [m] \}\]

The KKT conditions

- are necessary first-order optimality conditions
- are a lot more complicated than unconstrained optimization conditions
- extend to equality constraints (associated dual inequality constraints are always active)
- are also necessary with other (typically weaker) types of constraint qualification
- technically don’t require constraint qualification (Fritz-John conditions), but this makes them less useful
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