Numerical Optimization

Finding the best feasible solution

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Review: Unconstrained Optimization

- "Objective Function" or "Cost Function"
  - May be function of many variables
- Ex: $\min x^2 + y^2$
  - 2D problem defines manifold (surface) in 3D space
  - $z = x^2 + y^2$
- Must find point where gradient of function = 0

$$\nabla f(x,y) = \begin{bmatrix} \frac{\delta f}{\delta x} \\ \frac{\delta f}{\delta y} \end{bmatrix}$$

Question 1

$$f(x,y) = x^3 y^2$$

- **Question: What is equivalent to the gradient of the above function evaluated at the point $x=1, y=1$**
  - [A] $\begin{bmatrix} 3x \\ 2y \end{bmatrix}$ [B] $\begin{bmatrix} 3 \\ 2 \end{bmatrix}$ [C] $\begin{bmatrix} 3x^2y^2 \\ 2x^3y \end{bmatrix}$
  - [D] All of the above.
  - [E] I have no clue.
- Answer:
  - ???

Question 2

$$f(x,y) = 3x - 2y$$

- **Question: What is the gradient of the above function at $x=1, y=1$**
  - [A] $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ [B] $\begin{bmatrix} 3 \\ 2 \end{bmatrix}$ [C] $\begin{bmatrix} 3 \\ -2 \end{bmatrix}$
  - [D] All of the above.
  - [E] I have no clue.
- Answer:
  - ???

Review: Unconstrained Optimization

- For minimization, $-\nabla f$ points "downhill" in steepest direction
- Trick for maximization problems:

$$\max_{\underline{x}} f(\underline{x}) = \min_{\underline{x}} -f(\underline{x})$$

- Steepest Descent Method:
  - Start at initial guess, $\underline{x}_0$
  - Evaluate $-\nabla f$ at current point
  - Perform line search in improving direction
  - Update current best point and repeat until $-\nabla f$ is "small"

Review: Constrained Optimization

- Standard form with N constraints:

$$\begin{aligned} &\min_{\underline{x}} f(\underline{x}) \\ \textit{subject to } &g_1(\underline{x}) \leq 0 \\ &g_2(\underline{x}) \leq 0 \\ &\vdots \\ &g_N(\underline{x}) \leq 0 \end{aligned}$$

- Bounds on variables in standard form:

$$1 \leq x \leq 10$$

$$\begin{aligned} 1 - x &\leq 0 \\ x - 10 &\leq 0 \end{aligned}$$

Review: Constrained Optimization

- Standard form with N constraints:

$$\min_{\underline{x}} f(\underline{x})$$

$$\begin{aligned} \textit{subject to } g_1(\underline{x}) &\leq 0 \\ g_2(\underline{x}) &\leq 0 \\ &\vdots \\ g_N(\underline{x}) &\leq 0 \end{aligned}$$

- Equality constraints in standard form:

$$x = y^2$$

$$0 \leq x - y^2 \leq 0$$

$$\begin{aligned} x - y^2 &\leq 0 \\ -x + y^2 &\leq 0 \end{aligned}$$

Review: Linear vs. Nonlinear

- Linear examples and general form for sets of linear equality and inequality constraints:

$$\begin{aligned} 2x + 3y &= 4 \\ x - y &\leq 2 \end{aligned}$$

$$\begin{aligned} \underline{\underline{A}}\,\underline{x} &= \underline{b} \\ \underline{\underline{A}}\,\underline{x} &\leq \underline{b} \end{aligned}$$

- Nonlinear examples and general form for nonlinear constraints:

$$\begin{aligned} 2x^2 + y^2 &= 4 \\ y &= e^x \end{aligned}$$

$$\begin{aligned} g(\underline{x}) &\leq 0 \\ h(\underline{x}) &= 0 \end{aligned}$$

Review: Convex vs. Nonconvex

- Eigenvalues of Hessian must be ≥ 0 to be convex function
- Graphically: In a convex set you may pick any two points and the line between the two points contains only points inside the set.
- Get problem in standard form, check Hessian eigenvalues:

$$y \geq x^2$$
$$x^2 - y \leq 0$$

$$\nabla f(\underline{x}) = \begin{bmatrix} 2x \\ -1 \end{bmatrix} \quad H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial y \partial x} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$$

Eigenvalues are 2, 0 so $y \geq x^2$ is a convex constraint.

Review: Convex vs. Nonconvex

- Unconstrained example

$$\min_{x,y} x^2 + y^2$$

$$\nabla f(\underline{x}) = \begin{bmatrix} 2x \\ 2y \end{bmatrix} \quad H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial y \partial x} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

Eigenvalues are 2, 0 so $x^2 + y^2$ is a convex constraint.

Question 3

$$x^2 + y^2 \geq 9$$

- **Question: Is the constraint convex?**
  - [A] Yes
  - [B] No
  - [C] What?
  - [D] All of the above.
  - [E] I have no clue.
- Answer:
  - ???

Review: Convex vs. Nonconvex

- General form for constrained optimization:

$$\min_{\underline{x}} f(\underline{x})$$

$$\begin{aligned} \textit{subject to } g_1(\underline{x}) &\leq 0 \\ g_2(\underline{x}) &\leq 0 \\ h_1(\underline{x}) &= 0 \\ h_2(\underline{x}) &= 0 \end{aligned}$$

- **Rules. Nonconvex problem if any of following are true:**
  - $f(\underline{x})$ is a nonconvex function in the domain of $\underline{x}$
  - Any $g_i(\underline{x})$ inequality constraint is a nonconvex function in the domain of $\underline{x}$
  - Any $h_i(\underline{x})$ equality constraint is nonlinear
- **Convex problems have a single solution**

Question 4

$$\min_{x,y} \; -2x + y$$
$$x^2 + y^2 \leq 9$$

- **Question: Is the problem convex?**
  - [A] Yes
  - [B] No
  - [C] What?
  - [D] All of the above.
  - [E] I have no clue.
- Answer:
  - ???

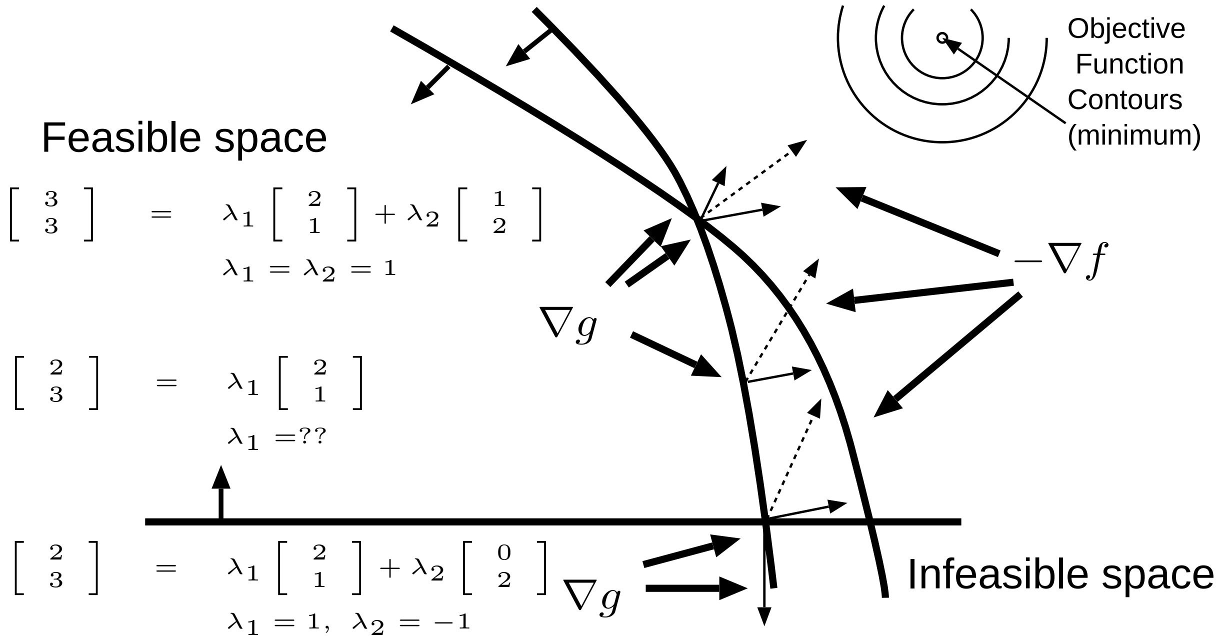
Review: KKT Conditions

- Check to see if a point $\underline{x}^*$ is optimal in constrained optimization
  - Put problem in standard form with only inequality constraints
  - Find any active constraints, $g_i(\underline{x}^*) = 0$
  - Solve for Lagrange multipliers

$$-\nabla f(\underline{x}^*) = \sum \lambda_i \, g_i(\underline{x}^*)$$
$$\lambda_i \geq 0$$

- Lagrange multipliers represent how "hard" the problem "pushes" against the constraints
- Lagrange multipliers must all be positive for the point to be a KKT point

Review: KKT Conditions



Question 5

$$\min_{x,y} x$$
$$x^2 + y^2 \leq 9$$

- **Question: Is the point $x = -3$, $y = 0$ a KKT point?**
  - [A] Yes
  - [B] No
  - [C] What?
  - [D] All of the above.
  - [E] I have no clue.
- Answer:
  - ???

Question 6

- **Question: Why do we care about optimization?**
  - [A] Gatzke told me to
  - [B] Model Predictive Control (MPC)
  - [C] Parameter estimation
  - [D] It is a useful tool for many problems
  - [E] All of the above
- Answer:
  - ???

Motivation: Process Design

- Objective function: Maximize profits, minimize cost
- Decision variables:
  - Number and size of components
  - Flow rates, temperatures, pressures
- Constraints
  - Mass and energy balances / design equations
  - Environmental limits, product limits

Motivation: Process Modeling

- Objective function: minimize the error between data and model
- Decision variables:
  - Model parameters (kinetic parameters)
- Constraints:
  - Model equations
  - Assumed limits on parameters
  - Physical limits on variables (concentrations positive)

Motivation: Process Scheduling

- Objective function: minimize the cost for your process
- Decision variables:
  - When to make products
  - What equipment to use
- Constraints:
  - Limits on batch sizes
  - Limits on storage
  - Order fulfillment requirements

Motivation: Process Control

- Objective function: minimize future deviation from setpoint
- Decision variables:
  - Future process input values
- Constraints:
  - Dynamic model equations for prediction
  - Limits on the inputs
  - Process variable limits

Problems: Linear Programming (LP)

Space for Notes Below

Problems: Quadratic Programming (QP)

Space for Notes Below

Problems: Nonlinear Programming (NLP)

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Problems: Mixed-Integer Linear Programming (MILP)

Space for Notes Below

Problems: Mixed-Integer Nonlinear Programming (MINLP)

Space for Notes Below

Question 7

$$\min_{x,y} \; -x$$
$$x^2 + y^2 \leq 9$$

- **Question: What kind of problem is this?**
  - [A] LP
  - [B] QP
  - [C] Convex NLP
  - [D] Nonconvex NLP
  - [E] MILP
- Answer:
  - ???

Question 8

$$\min_{x,y} \; -x$$
$$x + y \leq 9$$
$$y - x = 7$$

- **Question: What kind of problem is this?**
  - [A] LP
  - [B] QP
  - [C] Convex NLP
  - [D] Nonconvex NLP
  - [E] MILP
- Answer:
  - ???

Question 9

$$\min_{x,y} x^2 + y^2$$
$$x + 2y \leq 9$$

- **Question: What kind of problem is this?**
  - [A] LP
  - [B] QP
  - [C] Convex NLP
  - [D] Nonconvex NLP
  - [E] MILP
- Answer:
  - ???

LP / NLP / QP Solution Strategies

- Active set (simplex)
  - Pick set of active constraints
  - Solve problem in form $Ax = b$
  - Check to see if KKT holds
- Interior point
  - Put constraints into objective function
  - Find improving direction
  - Polynomial time algorithm

NLP / MILP / MINLP Stochastic Solution Strategies

- Genetic Algorithms
  - Make a "population" of random points,evaluate [0 1 1 0 0 1]
  - "Breed" based on resulting objective function values
  - "Mutate" some points randomly
- Simulated Annealing
  - Start at some initial guess
  - Search randomly nearby
  - As system "cools" limit search area
- Particle Swarm
  - Start with a random group of points
  - Get group information to move in better direction

Question 10

- **What is the most confusing optimization topic?**
  - [A] Convexity of functions / constraints
  - [B] KKT conditions
  - [C] Problem classification
  - [D] Solution strategies
  - [E] Other
- Answer:
  - ???