

Engineering Optimization

Concepts and Applications



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Contents

- Outline of remaining lectures
- Unconstrained problems
 - ...

Covered so far ...

1. Introduction:

- Negative null form
- Applications

2. Optimization problem:

- Definition
- Characteristics

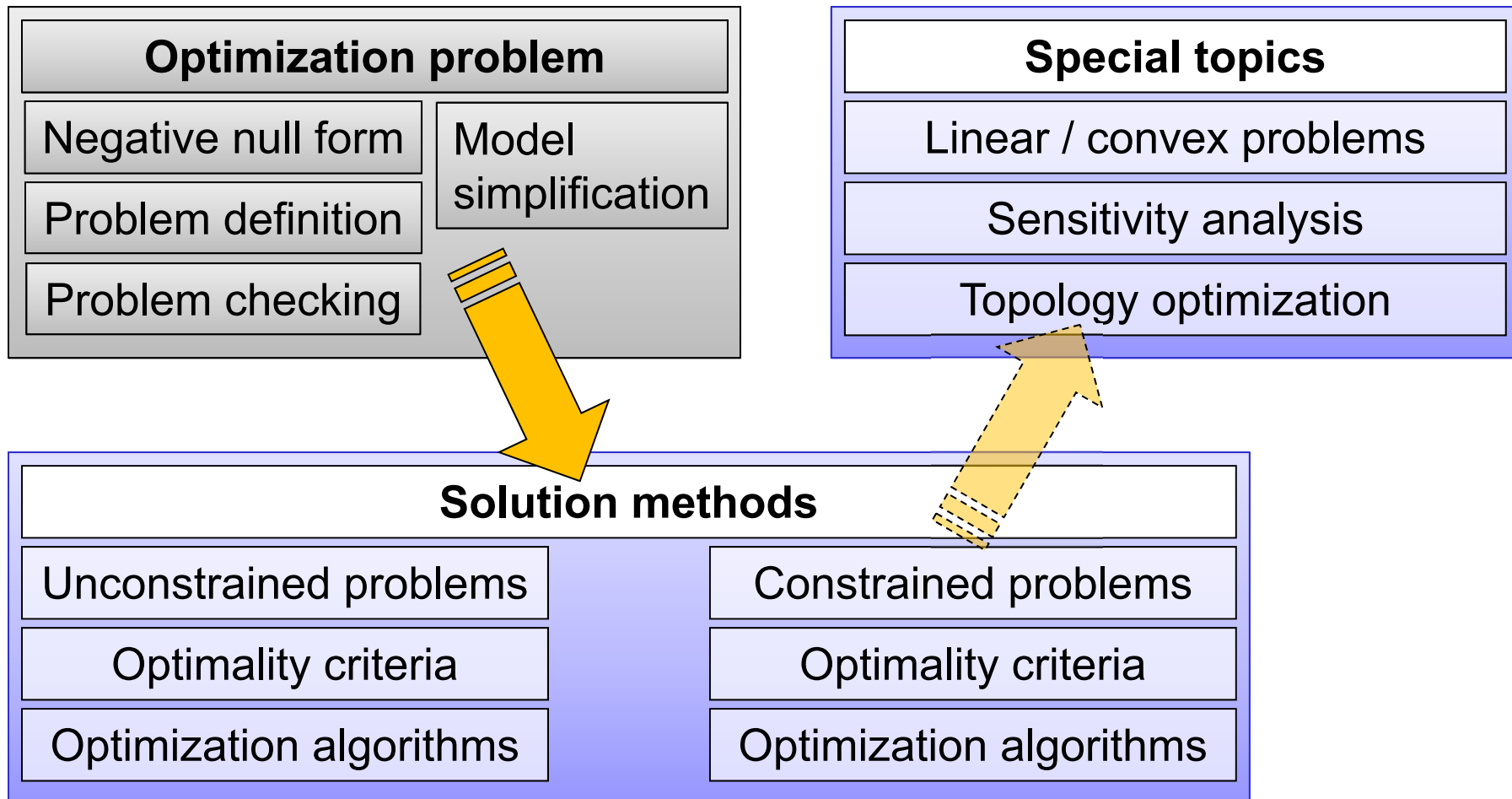
3. Problem checking:

- Boundedness
- Monotonicity analysis

4. Optimization model:

- Model simplification
- Approximation

Upcoming topics



Contents

- Outline of remaining lectures
- Unconstrained problems
 - Transformation methods
 - Existence of solutions, optimality conditions
 - Nature of stationary points
 - Global optimality

Unconstrained Optimization

- Why?

- Elimination of active constraints → unconstrained problem
- Develop basic understanding useful for constrained optimization
- Transformation of constrained problems into unconstrained problems
- Relevant engineering problems (potential energy minimization)

$$\min_{\mathbf{x}} f(\mathbf{x})$$
$$\underline{\mathbf{x}} \leq \mathbf{x} \leq \overline{\mathbf{x}}$$

Transforming constrained problem

- Reformulation through *barrier functions*:

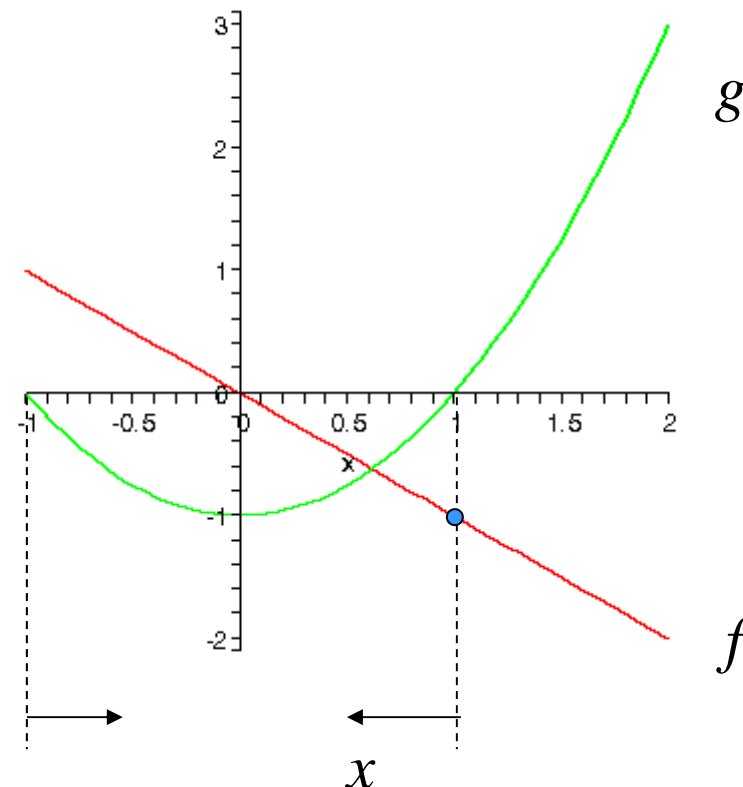
$$f = -x$$

$$g = x^2 - 1 \leq 0$$

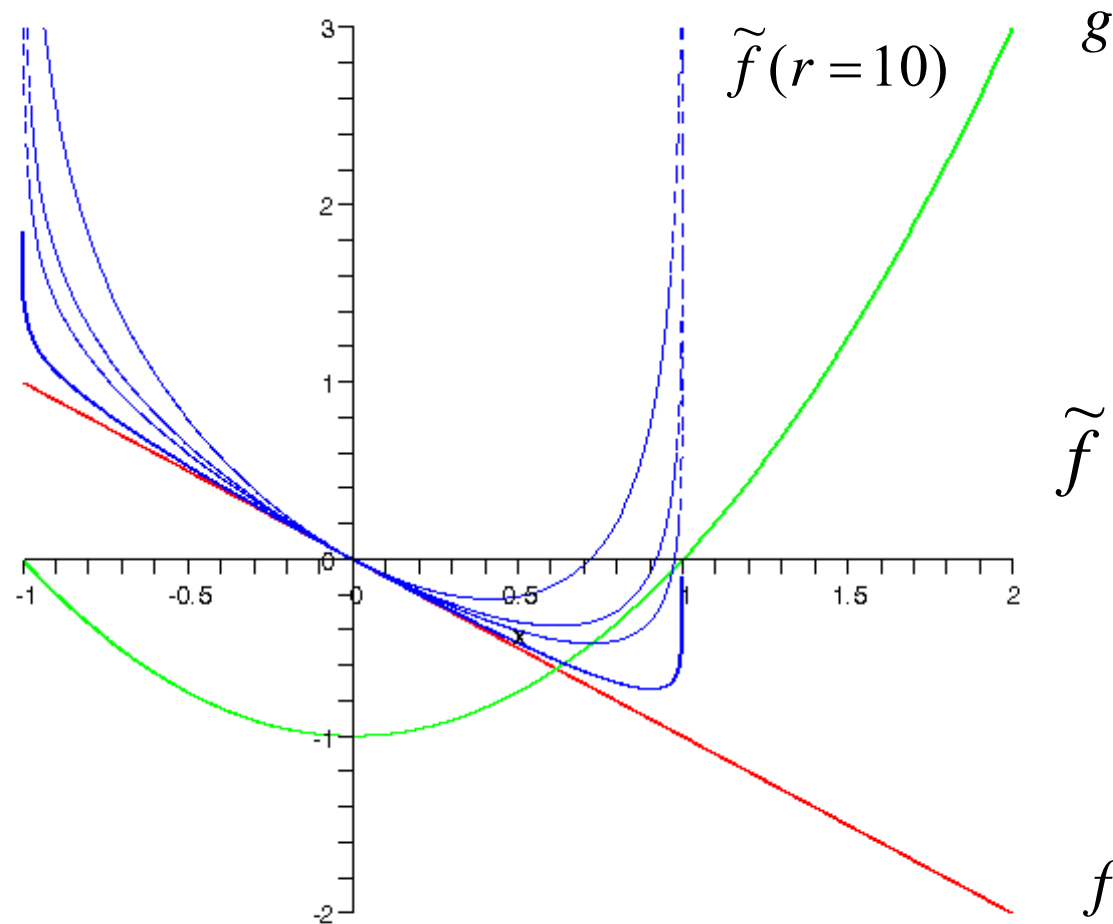
Transformation:

$$\tilde{f} = f - \frac{1}{r} \ln(-g)$$

$$\tilde{f} = -x - \frac{1}{r} \ln(1 - x^2)$$



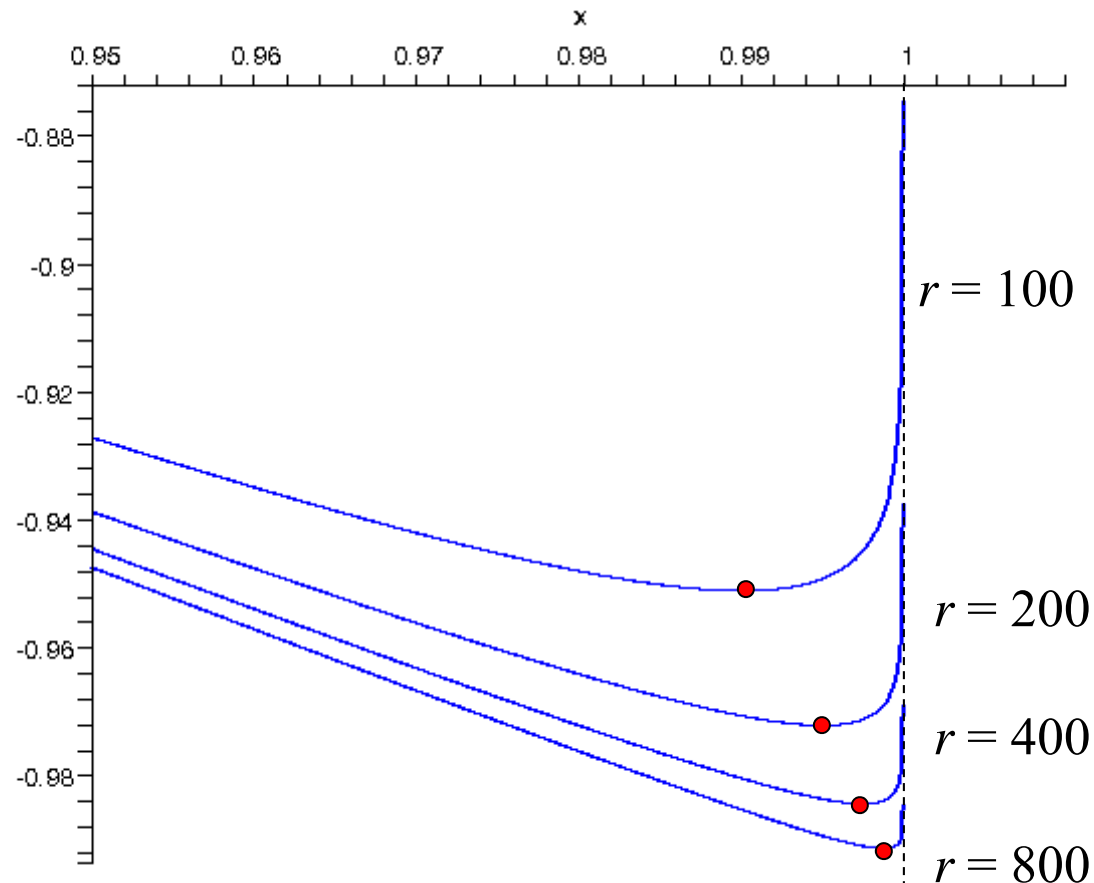
Transformed problem



$$\tilde{f} = f - \frac{1}{r} \ln(-g)$$

Transformed problem

- Barrier functions result in feasible, *interior* optimum:



Penalization



- Alternative reformulation: *penalty functions*

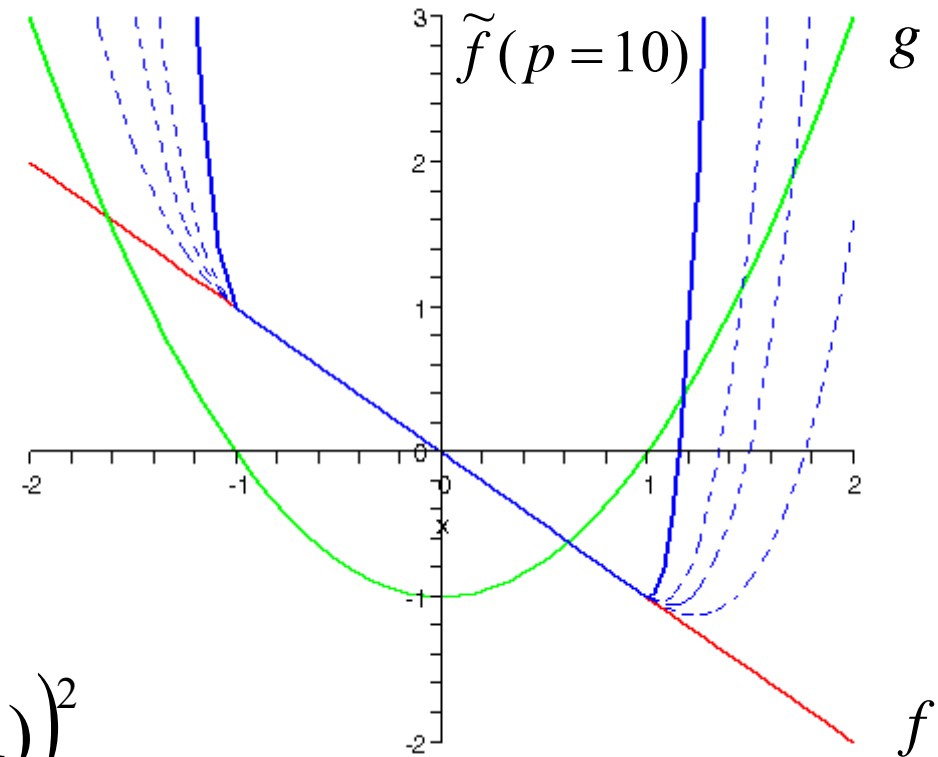
$$f = -x$$

$$g = x^2 - 1 \leq 0$$

Transformation:

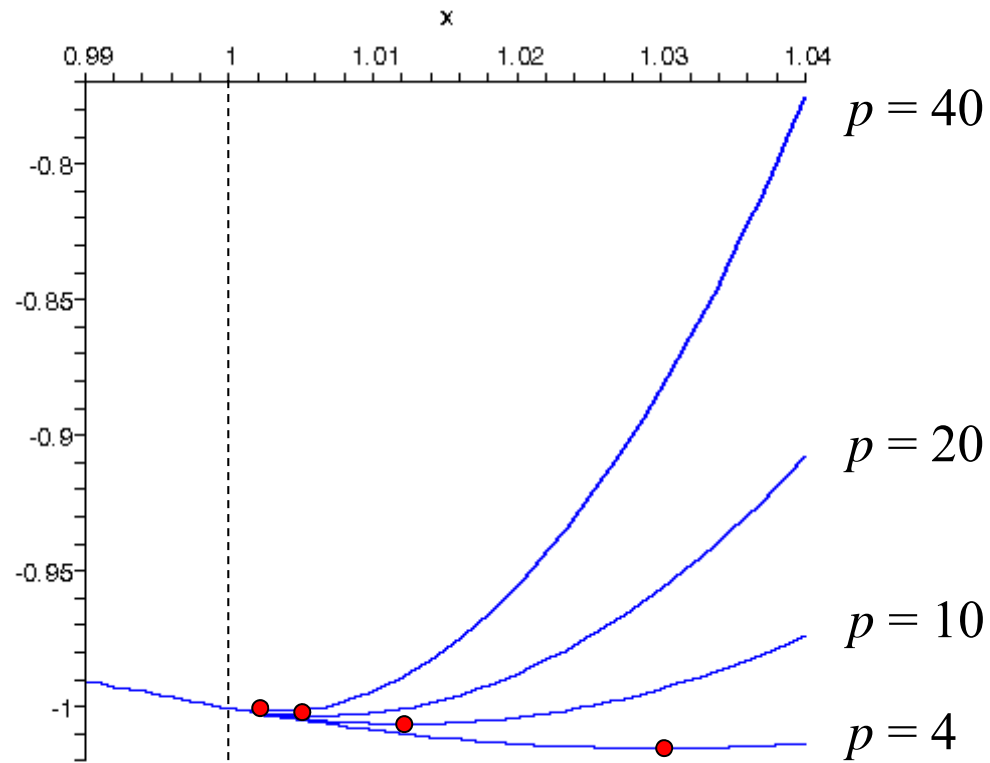
$$\tilde{f} = f + p(\max(0, g))^2$$

$$\tilde{f} = -x + p(\max(0, x^2 - 1))^2$$



Penalization (2)

- Penalty functions result in infeasible, *exterior* optimum:



Problem transformation summary

	Barrier function	Penalty function
Need feasible starting point?	Yes	No
Nature of optimum	Interior (feasible)	Exterior (infeasible)
Type of constraints	g	g, h

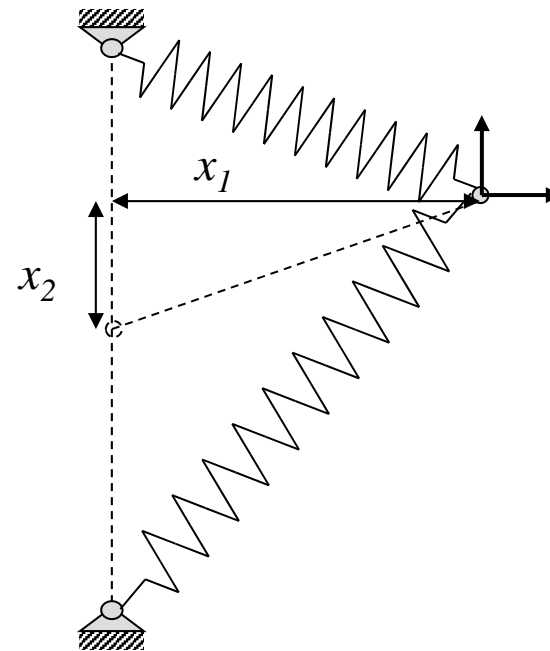
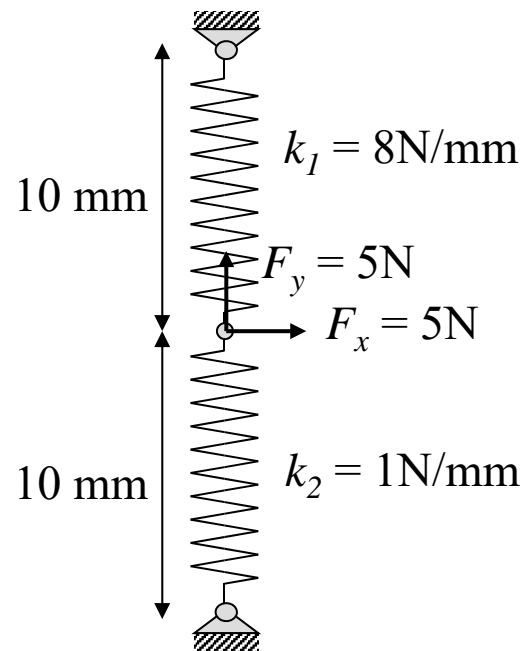
Generally constants r, p are iteratively increased to converge.

Unconstrained Optimization

- Why?
 - Elimination of active constraints → unconstrained problem
 - Develop basic understanding useful for constrained optimization
 - Transformation of constrained problems into unconstrained problems
 - Relevant engineering problems (potential energy minimization)

Unconstrained engineering problem

- Example: displacement of loaded structure



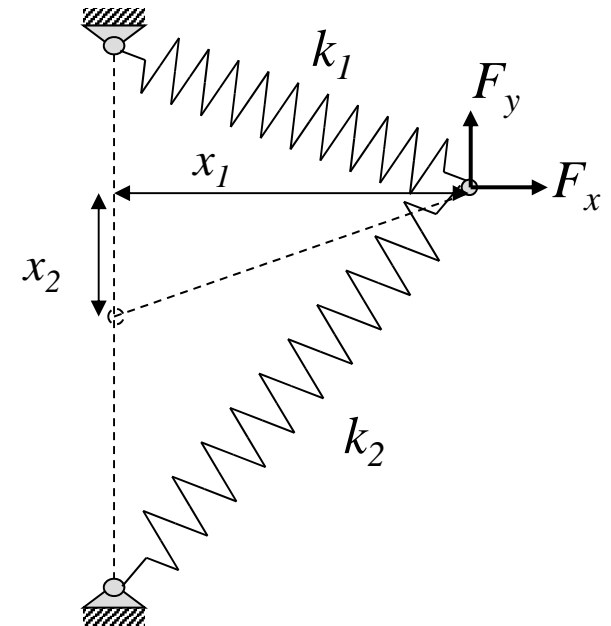
- Equilibrium: minimum potential energy

Unconstrained engineering problem

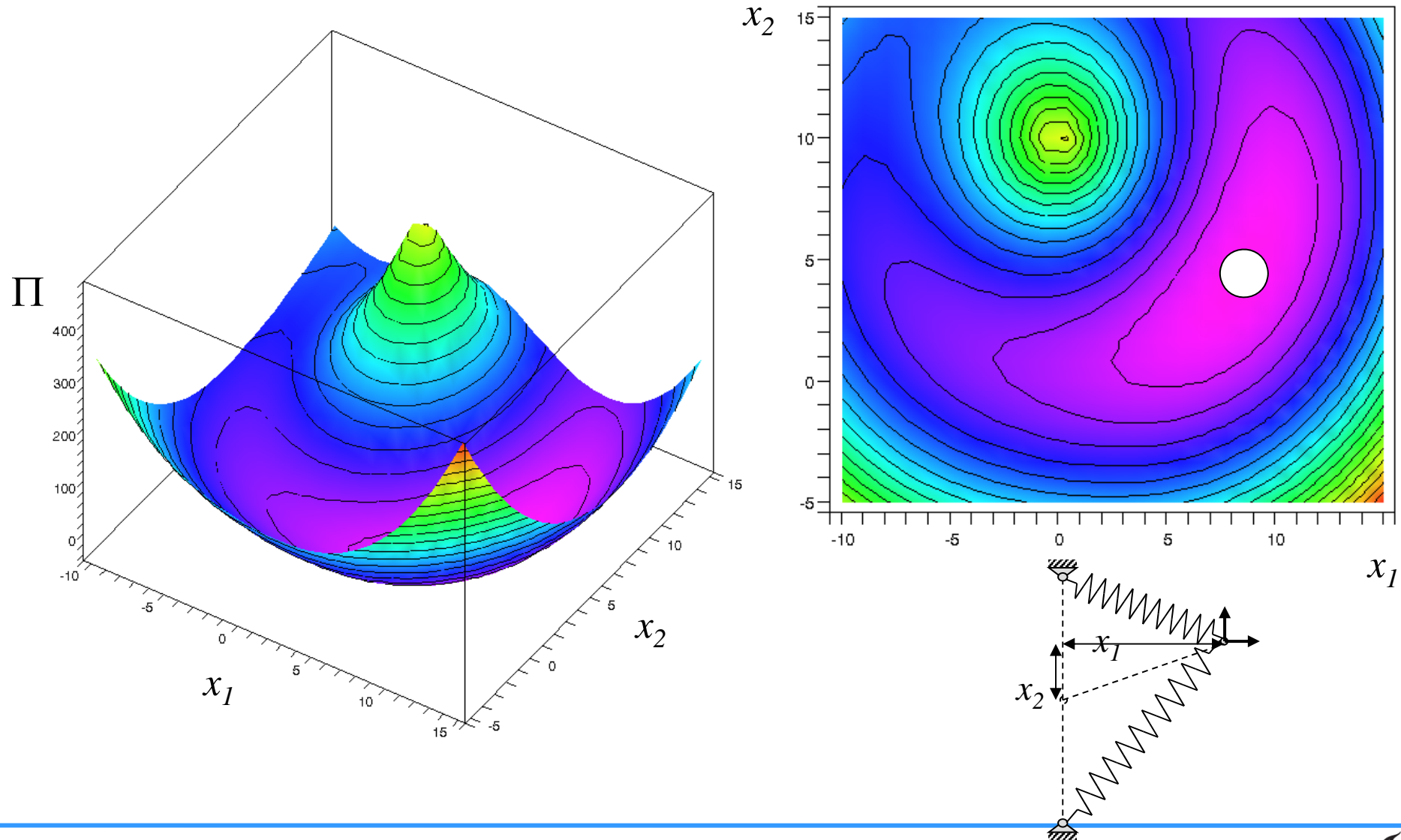
- Potential energy:

$$\begin{aligned}\Pi &= \frac{1}{2}k_1 u_1^2 + \frac{1}{2}k_2 u_2^2 - F_x x_1 - F_y x_2 \\ &= 4\left(\sqrt{x_1^2 + (10 - x_2)^2} - 10\right)^2 \\ &\quad + 0.5\left(\sqrt{x_1^2 + (10 + x_2)^2} - 10\right)^2 \\ &\quad - 5x_1 - 5x_2\end{aligned}$$

- Equilibrium: $\min_{x_1, x_2} \Pi$



Unconstrained engineering problem



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 - Existence of solutions, optimality conditions
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Significance of Optimality Conditions

Question:

Given a point \mathbf{x}^* , how can we determine if it is a minimizer?

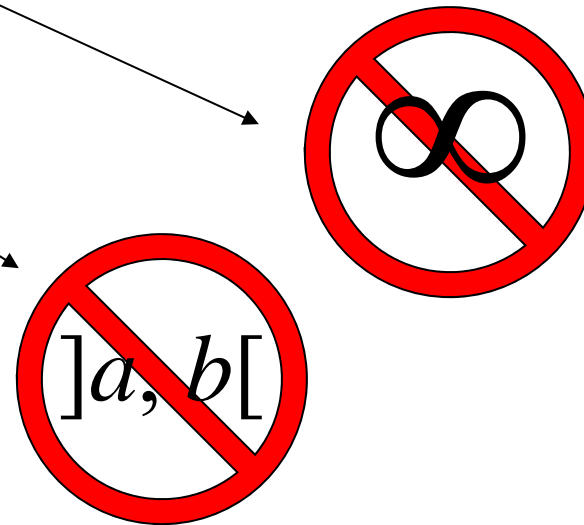
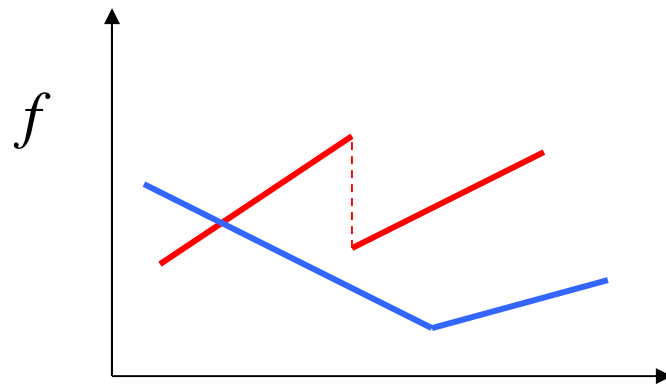
i.e. How to recognize/identify an optimal point?



Answer: Check **optimality conditions at point \mathbf{x}^*** .

Theory for solving unconstrained optimization problems

- Assumptions:
 - Objective *continuous* and *differentiable* (C^1)
 - Domain *closed* and *bounded* (compact)





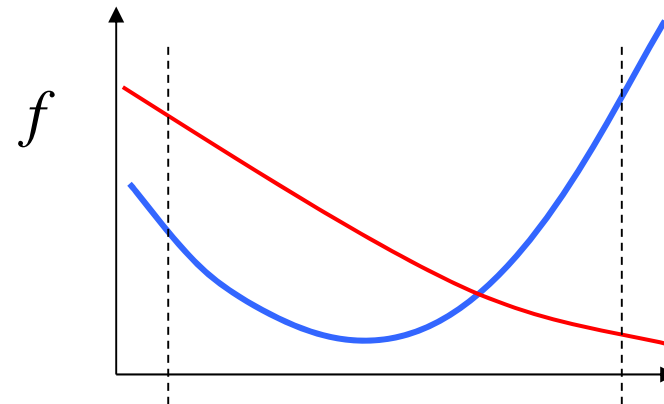
Existence of minima

- Weierstrass Theorem:

*“A **continuous** function on a **compact** set has a maximum and a minimum in that set”*

- *Sufficient* condition for existence!
- *Interior* optima only exist for *non-monotonic* functions

- Compact set: use \leq , not $<$ in constraints!

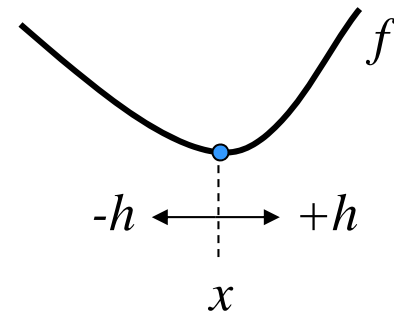


One-dimensional case

- Calculus: conditions for local minimum of f
 - Derivative zero: $f' = 0$ (necessary)
 - Second derivative positive: $f'' > 0$ (sufficient)
- Interpretation through Taylor series:

$$f(x+h) = f + f'h + o(h^2)$$

$$\left. \begin{aligned} \Delta f &= f(x+h) - f = f'h + o(h^2) \geq 0 \\ \Delta f &= f(x-h) - f = -f'h + o(h^2) \geq 0 \end{aligned} \right\} \Rightarrow f' = 0$$



One-dimensional case (2)

- Condition for local minimum: $f''(x) > 0$

$$\left. \begin{aligned} \Delta f = f(x+h) - f &= \frac{1}{2} f'' h^2 + o(h^3) > 0 \\ \Delta f = f(x-h) - f &= \frac{1}{2} f'' h^2 + o(h^3) > 0 \end{aligned} \right\} \Rightarrow f'' > 0$$

- Other possibilities:

$$f''(x) < 0$$

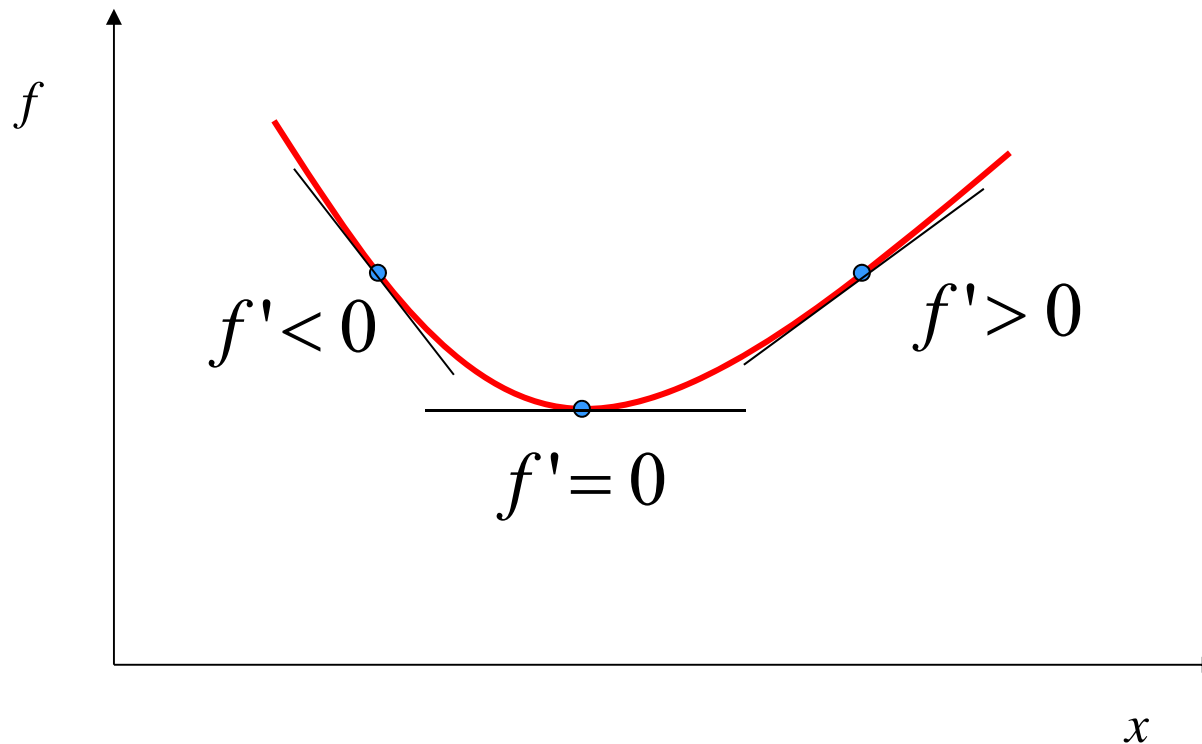
maximum

$$f''(x) = 0$$

? Check higher order derivatives

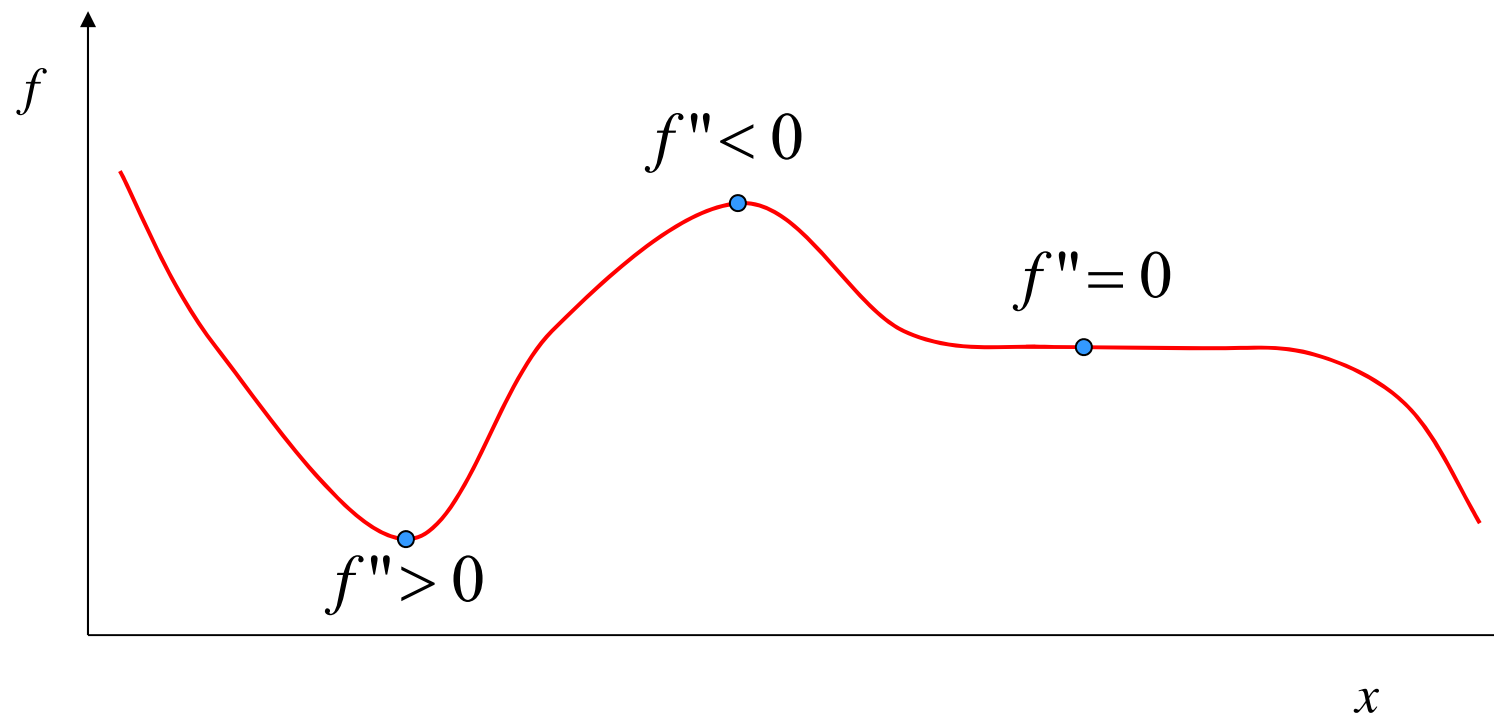
Geometrical interpretation

- Positive $f'' \Leftrightarrow f'$ locally increasing



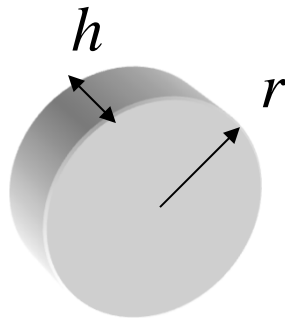
One-dimensional case (3)

- Possible situations for stationary points ($f' = 0$):



Example

- Aspirin pill revisited: “longest-lasting candy”
 - *Maximize* dissolving time \rightarrow minimize surface area



\Rightarrow

$$\min_{r,h} 2\pi r^2 + 2\pi r h$$

$$\text{s.t. } \pi r^2 h = 1$$



- Equality constraint active \rightarrow eliminate h

$$h = \frac{1}{\pi r^2} \quad \Rightarrow \quad \min_r 2\pi r^2 + \frac{2}{r}$$

Example (2)

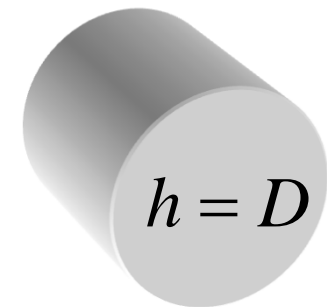
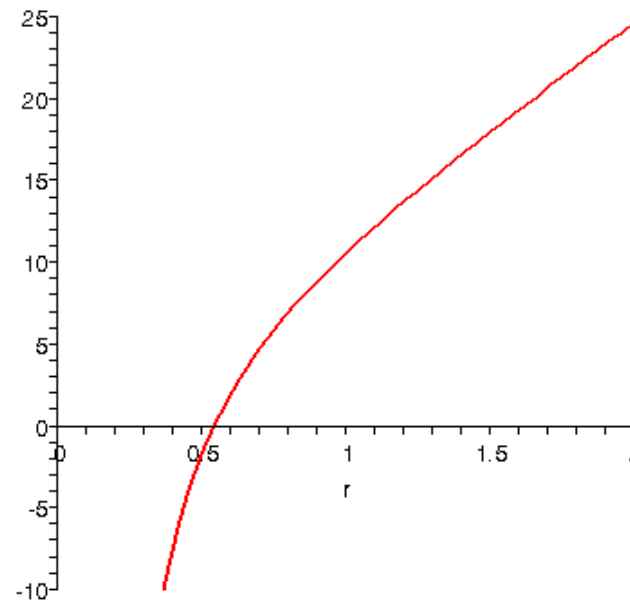
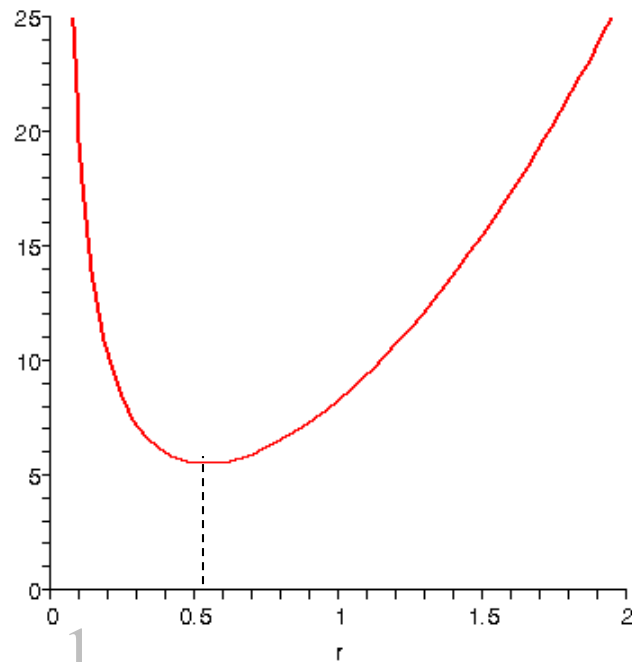


$$f = 2\pi r^2 + \frac{2}{r}$$

$$f' = 4\pi r - \frac{2}{r^2} = 0$$

$$f'' = 4\pi + \frac{4}{r^3}$$

$$> 0 \quad \forall r > 0$$

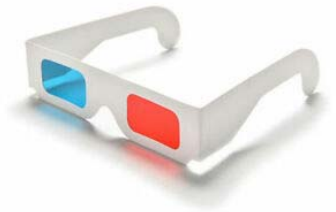


$$h = \frac{1}{\pi r^2}$$

$$r = (2\pi)^{-\frac{1}{3}} \approx 0.542$$

$$h = \frac{(2\pi)^{\frac{2}{3}}}{\pi} \approx 2r$$

Multidimensional case



- Local approximation to multidimensional minimum by multidimensional Taylor series:

$$f(\mathbf{x} + \mathbf{h}) = f + \nabla f^T \mathbf{h} + o(\|\mathbf{h}\|^2)$$

Gradient $\nabla f = \begin{Bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{Bmatrix}$

$$f(\mathbf{x} + \mathbf{h}) - f = \nabla f^T \mathbf{h} + o(\|\mathbf{h}\|^2) \geq 0$$

$$f(\mathbf{x} - \mathbf{h}) - f = -\nabla f^T \mathbf{h} + o(\|\mathbf{h}\|^2) \geq 0$$

(For any \mathbf{h})

Condition for minimum: $\nabla f = \mathbf{0}$

Multidimensional case (2)

- For minimum, consider second-order approximation:

$$f(\mathbf{x} + \mathbf{h}) = f + \nabla f^T \mathbf{h} + \frac{1}{2} \mathbf{h}^T \mathbf{H} \mathbf{h} + \mathcal{O}(\|\mathbf{h}\|^3)$$

Hessian $\mathbf{H} =$

$$\begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \ddots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \dots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Multidimensional case (3)

- Second order approximation:

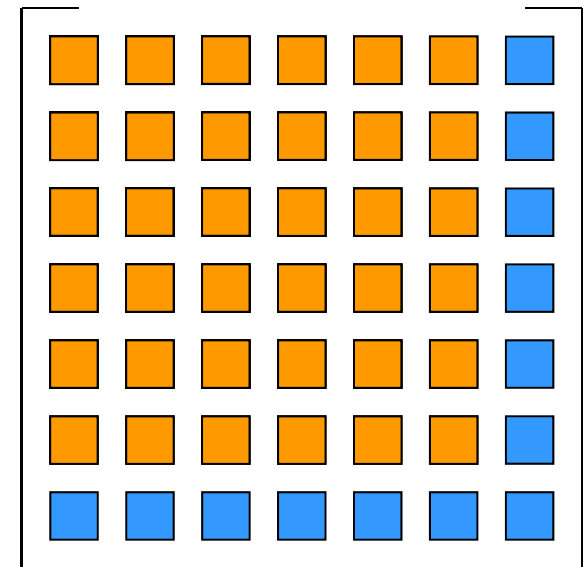
$$\left. \begin{aligned} f(\mathbf{x} + \mathbf{y}) - f &= \frac{1}{2} \mathbf{y}^T \mathbf{H} \mathbf{y} + o(\|\mathbf{y}\|^3) > 0 \\ f(\mathbf{x} + \mathbf{z}) - f &= \frac{1}{2} \mathbf{z}^T \mathbf{H} \mathbf{z} + o(\|\mathbf{z}\|^3) > 0 \\ f(\mathbf{x} + \mathbf{q}) - f &= \frac{1}{2} \mathbf{q}^T \mathbf{H} \mathbf{q} + o(\|\mathbf{q}\|^3) > 0 \end{aligned} \right\} \mathbf{y}^T \mathbf{H} \mathbf{y} > 0 \quad \forall \mathbf{y} \neq \mathbf{0}$$

- Local minimum: ***Optimality Conditions:***

- First Order Necessity Condition: $\nabla f = \mathbf{0}$
- Second Order Sufficiency Condition: $\mathbf{y}^T \mathbf{H} \mathbf{y} > 0 \quad \forall \mathbf{y}$

Positive definiteness

- $\mathbf{y}^T \mathbf{H} \mathbf{y} > 0 \quad \forall \mathbf{y} \neq \mathbf{0} \quad \Leftrightarrow \quad \text{Hessian } \textit{positive definite}$
- Tests for positive definiteness:
 - Evaluate $\mathbf{y}^T \mathbf{H} \mathbf{y}$ for all \mathbf{y} (impractical)
 - All *eigenvalues* λ_i of \mathbf{H} positive
 - Sylvester's rule: all determinants of \mathbf{H} and its *principal submatrices* are positive



Example

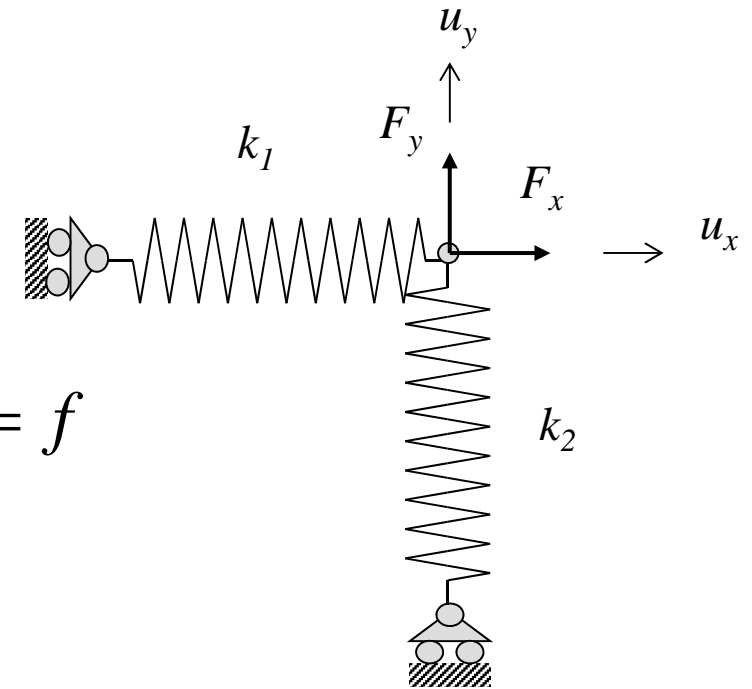
- Another loaded structure (small displacements):

$$\Pi = \frac{1}{2} k_1 u_x^2 + \frac{1}{2} k_2 u_y^2 - F_x u_x - F_y u_y = f$$

- Equilibrium: $\min_{u_x, u_y} f$

- First order necessity condition:

$$\nabla f = \begin{Bmatrix} \frac{\partial f}{\partial u_x} \\ \frac{\partial f}{\partial u_y} \end{Bmatrix} = \begin{Bmatrix} k_1 u_x - F_x \\ k_2 u_y - F_y \end{Bmatrix} = 0 \Rightarrow \begin{Bmatrix} u_x \\ u_y \end{Bmatrix} = \begin{Bmatrix} \frac{F_x}{k_1} \\ \frac{F_y}{k_2} \end{Bmatrix}$$



Example (2)

- Second order sufficiency: \mathbf{H} positive definite?

$$f = \frac{1}{2}k_1 u_x^2 + \frac{1}{2}k_2 u_y^2 - F_x u_x - F_y u_y \quad \nabla f = \begin{Bmatrix} k_1 u_x - F_x \\ k_2 u_y - F_y \end{Bmatrix}$$

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial u_x^2} & \frac{\partial^2 f}{\partial u_x \partial u_y} \\ \frac{\partial^2 f}{\partial u_y \partial u_x} & \frac{\partial^2 f}{\partial u_y^2} \end{bmatrix} = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix} \Rightarrow \begin{cases} k_1 > 0 \\ k_2 > 0 \end{cases}$$



Multidimensional quadratic functions

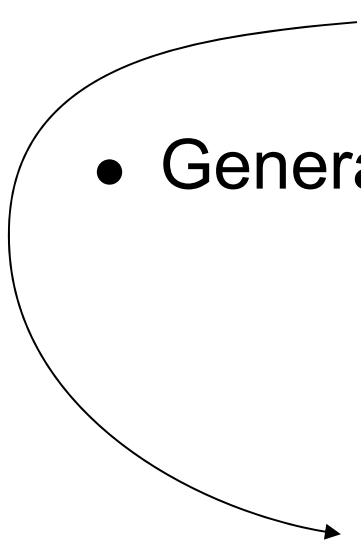
(for geometrical interpretation of optimality conditions)

- Polynomial terms up to 2nd order:

$$f(x_1, x_2, x_3) = 3 + 4x_2 + 2x_1x_2 - x_1^2 + x_3^2$$

- General form:

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + c$$


$$\frac{1}{2} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix}^T \begin{bmatrix} -2 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} + \begin{Bmatrix} 0 \\ 4 \\ 0 \end{Bmatrix}^T \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} + 3$$

- Note: 2nd order Taylor series is *exact*

Quadratic functions (2)

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{x} + c$$

- Optimality conditions:

- Gradient: $\nabla f = \mathbf{A} \mathbf{x} + \mathbf{b} = 0$

- Hessian: $\mathbf{H} = \mathbf{A}$

- Stationary points: $\mathbf{x} = -\mathbf{A}^{-1} \mathbf{b}$

1D: compare

$$f(x) = ax^2 + bx + c$$

$$x = -\frac{b}{2a} \quad \left(a = \frac{1}{2} \mathbf{A} \right)$$

Example

- Consider $f(\mathbf{x}) = \frac{1}{2} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix}^T \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} + \begin{Bmatrix} -1 \\ 4 \end{Bmatrix}^T \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} + 2$

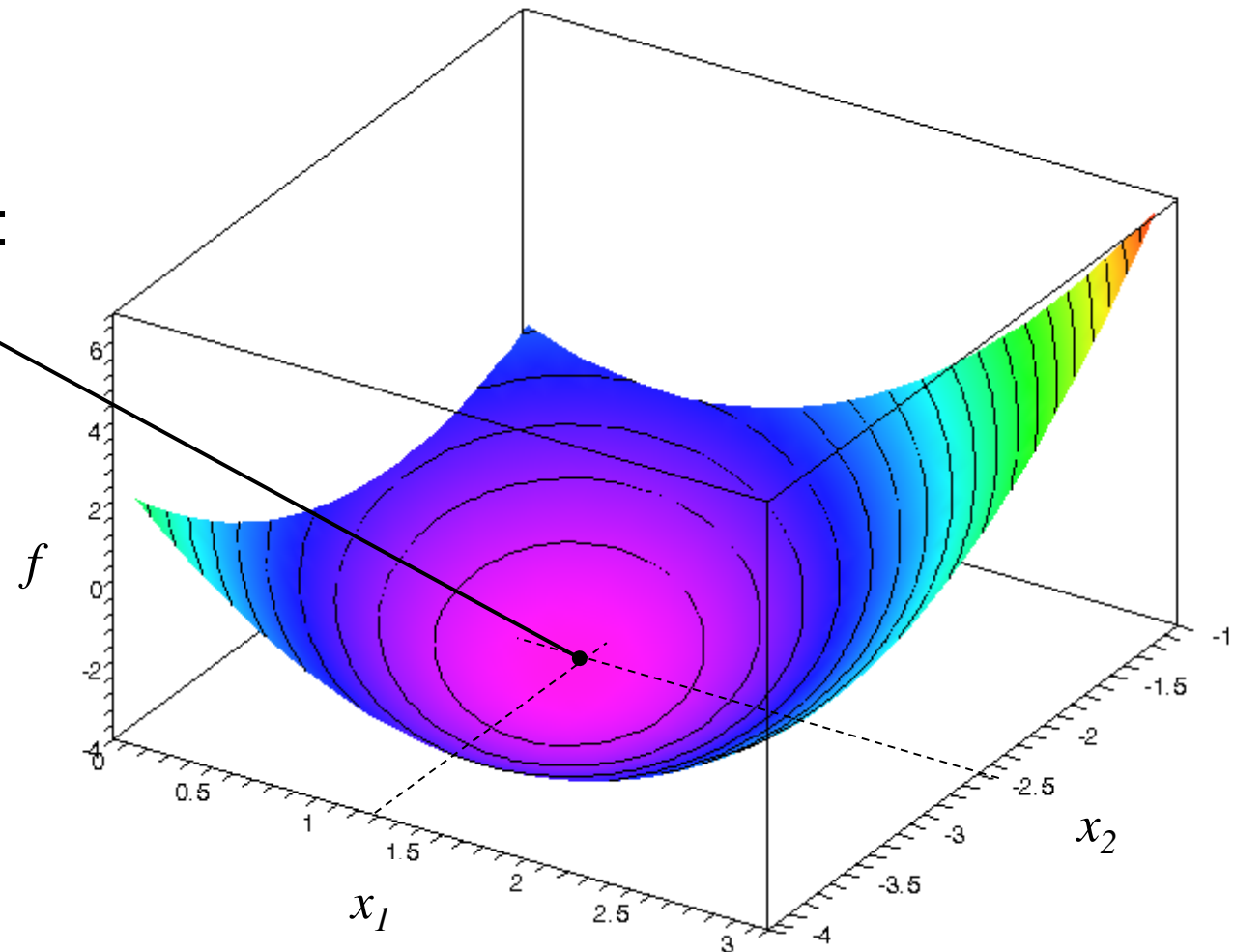
$$\Rightarrow \nabla f = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} + \begin{Bmatrix} -1 \\ 4 \end{Bmatrix} = \mathbf{0}$$

$$\Rightarrow \mathbf{x}^* = - \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix}^{-1} \begin{Bmatrix} -1 \\ 4 \end{Bmatrix} = \begin{Bmatrix} 1.2 \\ -2.6 \end{Bmatrix} \quad \text{Stationary point}$$

$$\mathbf{H} = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \Rightarrow \begin{cases} 3 > 0 \\ |\mathbf{H}| = 6 - 1 > 0 \end{cases} \quad \text{Hessian positive definite}$$

Example (2)

- Result:
minimum
at $(1.2, -2.6)$:



Example: least squares (Lect. 4)

- Least squares fitting: unconstrained optimization problem

$$\begin{aligned}\min_{\mathbf{a}} L &= \boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon} = (\tilde{\mathbf{f}} - \mathbf{M}\mathbf{a})^T (\tilde{\mathbf{f}} - \mathbf{M}\mathbf{a}) \\ \Rightarrow f(\mathbf{a}) &= \frac{1}{2} \mathbf{a}^T \underbrace{(2\mathbf{M}^T \mathbf{M})}_{\mathbf{A}} \mathbf{a} - \underbrace{2\tilde{\mathbf{f}}^T \mathbf{M}}_{\mathbf{b}^T} \mathbf{a} + \underbrace{\tilde{\mathbf{f}}^T \tilde{\mathbf{f}}}_{c}\end{aligned}$$

- Stationary point:

$$\begin{aligned}\mathbf{x} &= -\mathbf{A}^{-1} \mathbf{b} \\ \Rightarrow \mathbf{a} &= -\left(2\mathbf{M}^T \mathbf{M}\right)^{-1} \cdot -2\mathbf{M}^T \tilde{\mathbf{f}} \\ &= \left(\mathbf{M}^T \mathbf{M}\right)^{-1} \mathbf{M}^T \tilde{\mathbf{f}} \quad \checkmark\end{aligned}$$

- Hessian:

$$\begin{aligned}\mathbf{y}^T \mathbf{A} \mathbf{y} &= \mathbf{y}^T \left(2\mathbf{M}^T \mathbf{M}\right) \mathbf{y} \\ &= 2\left(\mathbf{M} \mathbf{y}\right)^T \left(\mathbf{M} \mathbf{y}\right) = 2\mathbf{z}^T \mathbf{z} > 0 \quad \checkmark\end{aligned}$$

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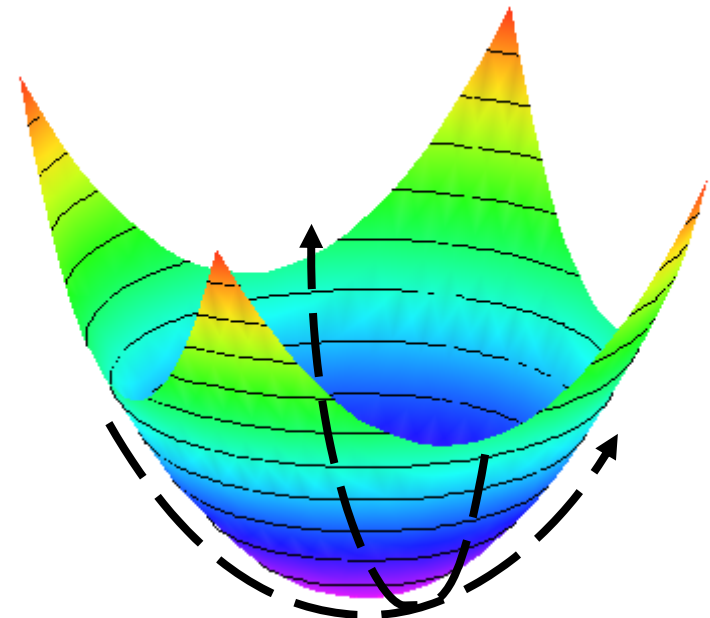
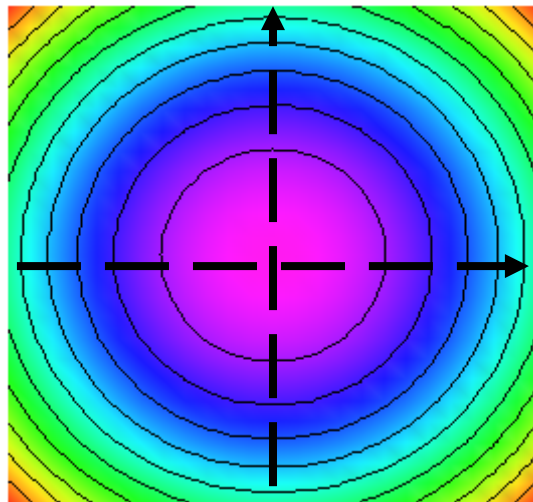
Nature of stationary points

- Hessian \mathbf{H} *positive definite*:

- Quadratic form $\mathbf{y}^T \mathbf{H} \mathbf{y} > 0$

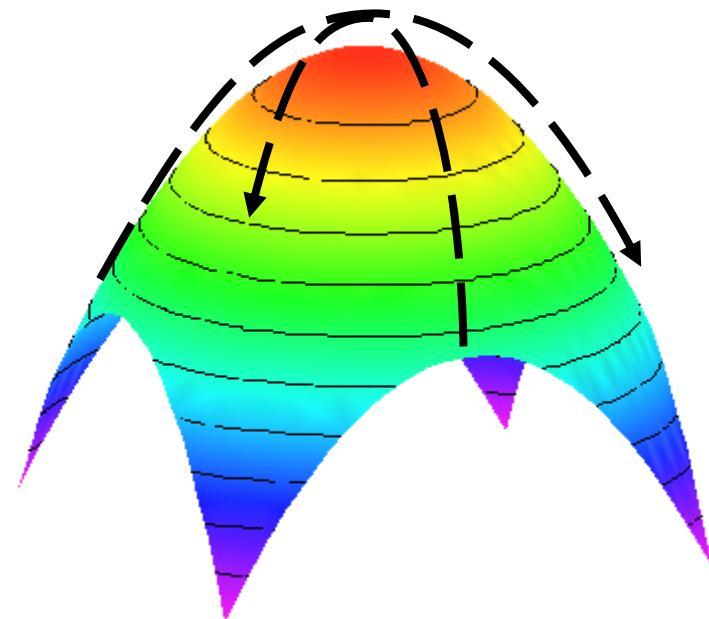
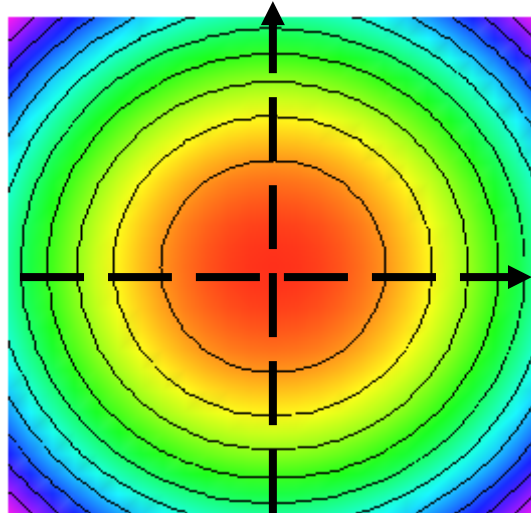
- Eigenvalues $\lambda_i > 0$ (\approx curvature)

- Local nature: (local) *minimum*



Nature of stationary points (2)

- Hessian \mathbf{H} *negative definite*:
 - Quadratic form $\mathbf{y}^T \mathbf{H} \mathbf{y} < 0$
 - Eigenvalues $\lambda_i < 0$
- Local nature: (local) *maximum*



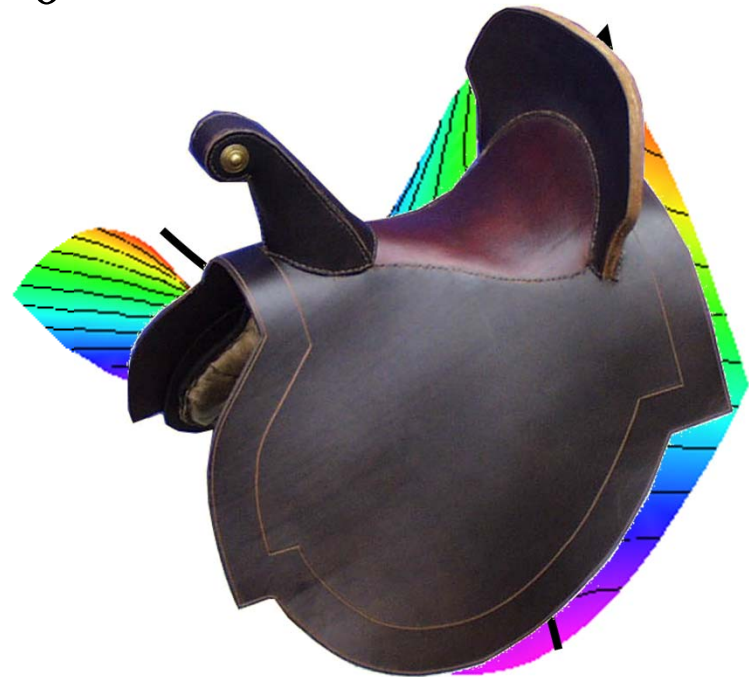
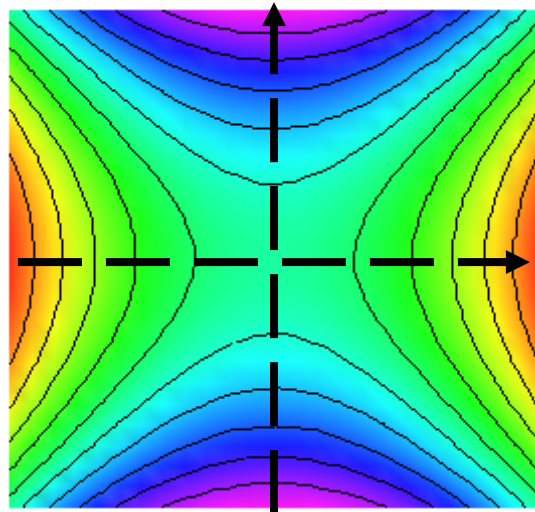
Nature of stationary points (3)

- Hessian \mathbf{H} *indefinite*:

- Quadratic form $\mathbf{y}^T \mathbf{H} \mathbf{y} \neq 0$

- Eigenvalues $\lambda_i \neq 0$

- Local nature: *saddle point*



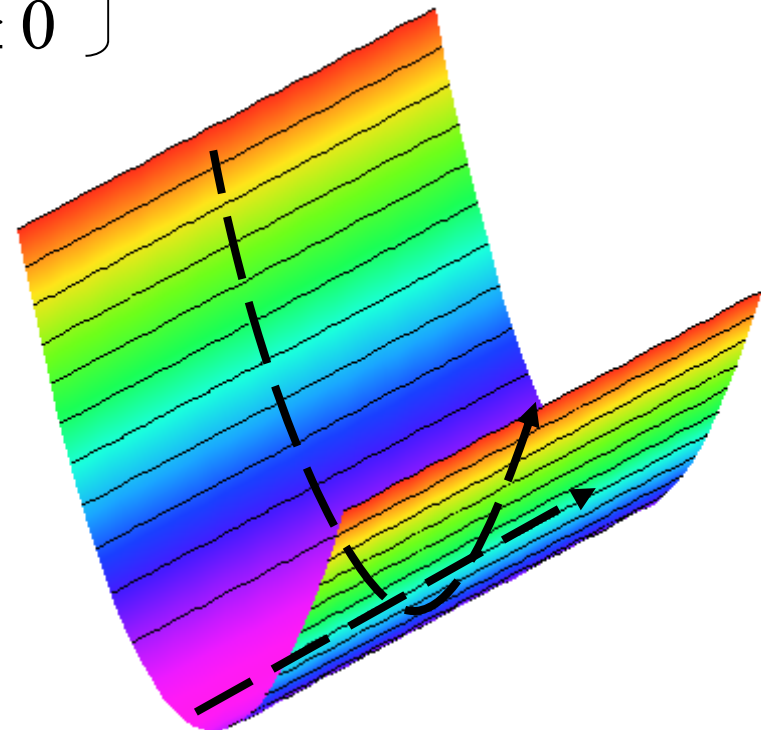
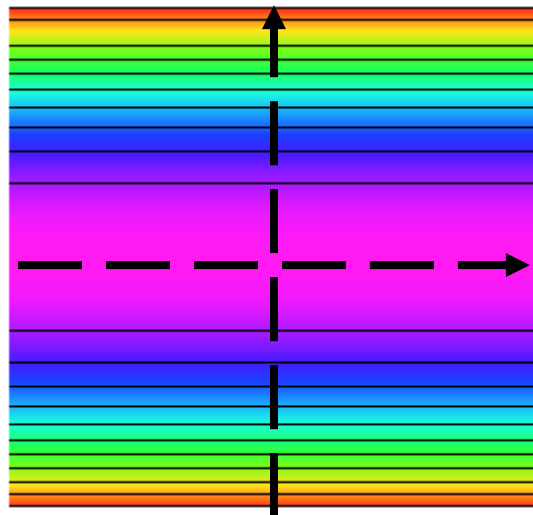
Nature of stationary points (4)

- Hessian \mathbf{H} *positive semi-definite*:

- Quadratic form
- Eigenvalues

$$\left. \begin{array}{l} \mathbf{y}^T \mathbf{H} \mathbf{y} \geq 0 \\ \lambda_i \geq 0 \end{array} \right\} \rightarrow \mathbf{H} \text{ singular}$$

- Local nature: *valley*



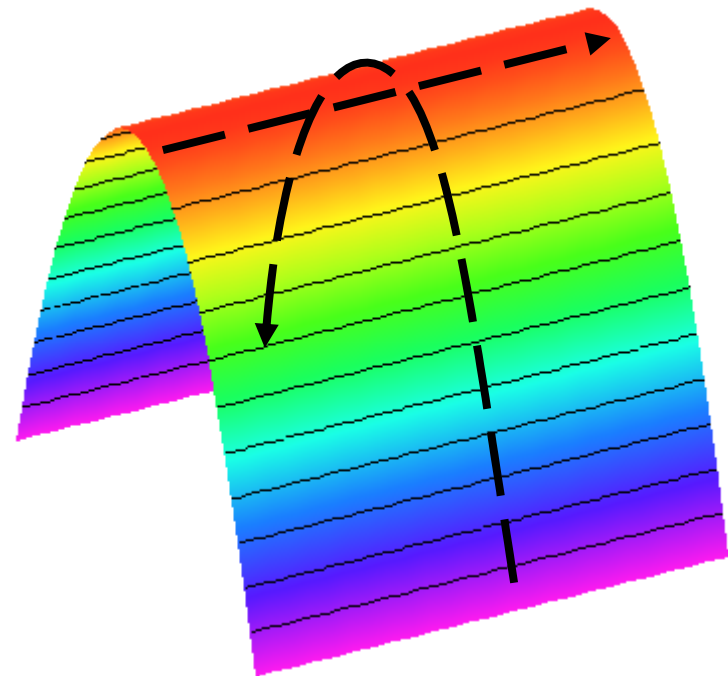
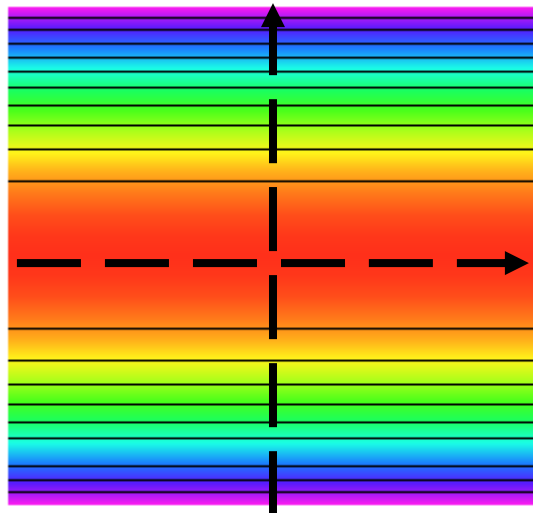
Nature of stationary points (5)

- Hessian \mathbf{H} *negative semi-definite*:

- Quadratic form
- Eigenvalues

$$\left. \begin{array}{l} \mathbf{y}^T \mathbf{H} \mathbf{y} \leq 0 \\ \lambda_i \leq 0 \end{array} \right\} \longrightarrow \mathbf{H} \text{ singular}$$

- Local nature: *ridge*



Stationary point nature summary

$$\underbrace{\mathbf{y}^T \mathbf{H} \mathbf{y}, \lambda_i}$$

$$> 0$$

Definiteness H

Positive d.

Nature \mathbf{x}^*

Minimum

$$\geq 0$$

Positive semi-d.

Valley

$$\neq 0$$

Indefinite

Saddlepoint

$$\leq 0$$

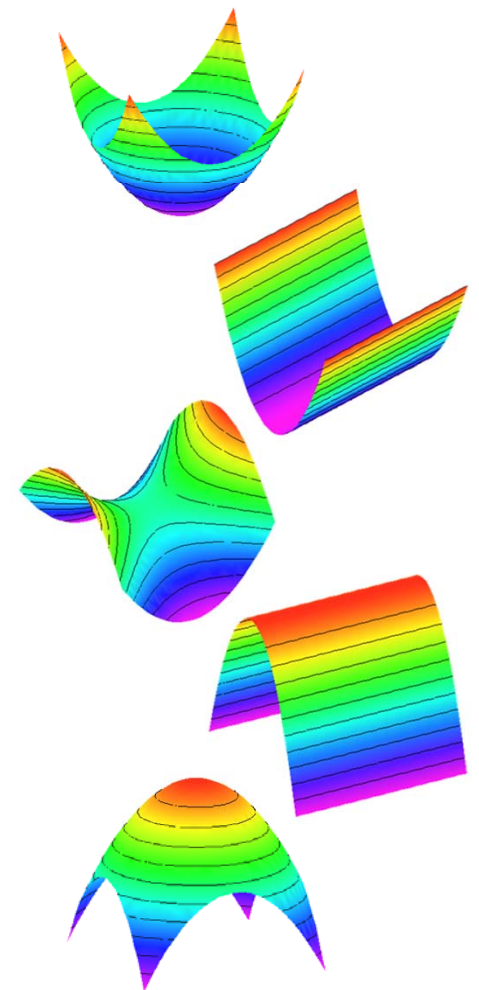
Negative semi-d.

Ridge

$$< 0$$

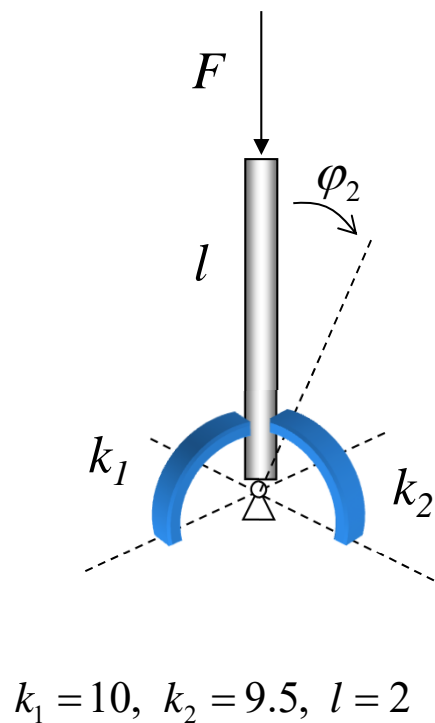
Negative d.

Maximum



Structural example: pin-jointed bar with rotational springs

- Nature of initial position depends on load (buckling):



$$dz = l - l \cos \varphi_1 \cos \varphi_2$$

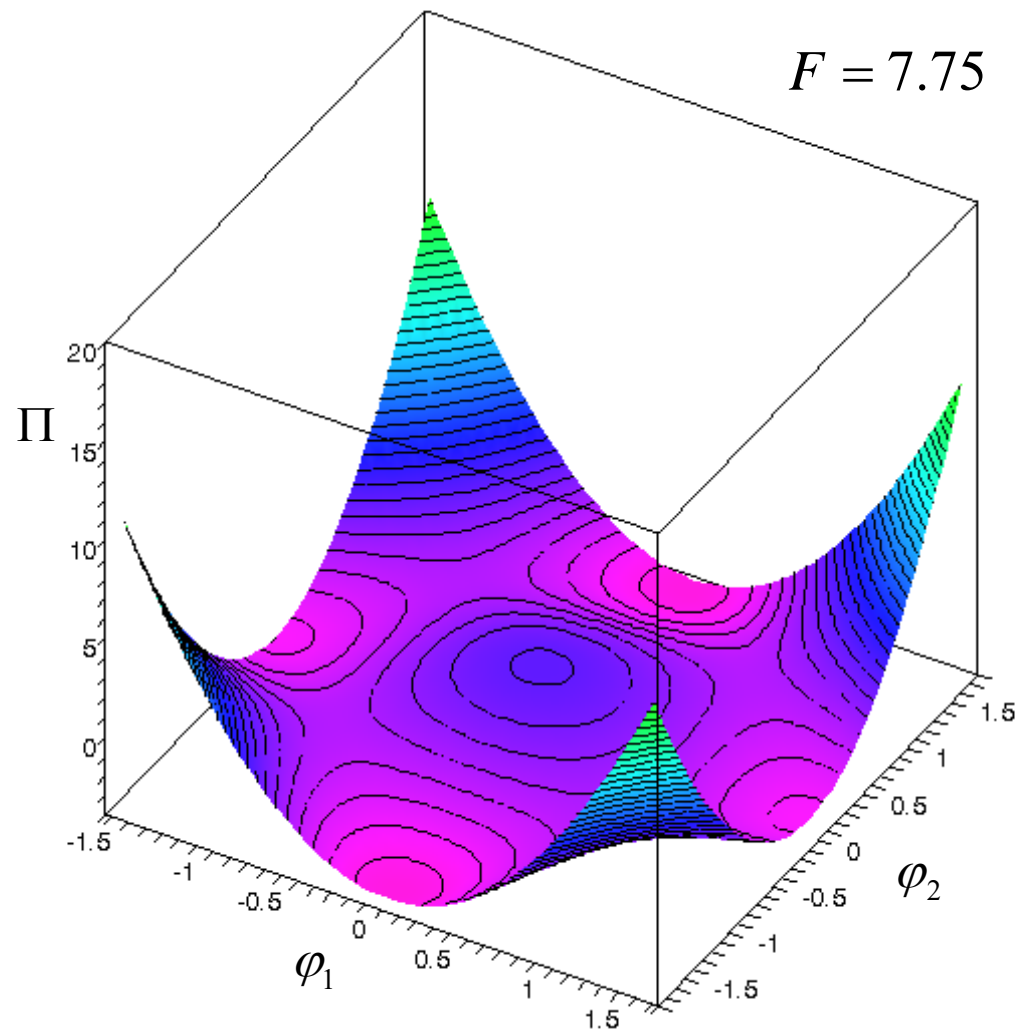
$$\Pi = \frac{1}{2} k_1 \varphi_1^2 + \frac{1}{2} k_2 \varphi_2^2 - F dz$$

$$\nabla \Pi = \begin{Bmatrix} k_1 \varphi_1 - Fl \sin \varphi_1 \cos \varphi_2 \\ k_2 \varphi_2 - Fl \sin \varphi_2 \cos \varphi_1 \end{Bmatrix} = \mathbf{0} \Rightarrow \varphi = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$$

$$\Delta \Pi = \begin{bmatrix} k_1 - Fl & 0 \\ 0 & k_2 - Fl \end{bmatrix} \Rightarrow F_{crit} = \min \left(\frac{k_1}{l}, \frac{k_2}{l} \right)$$

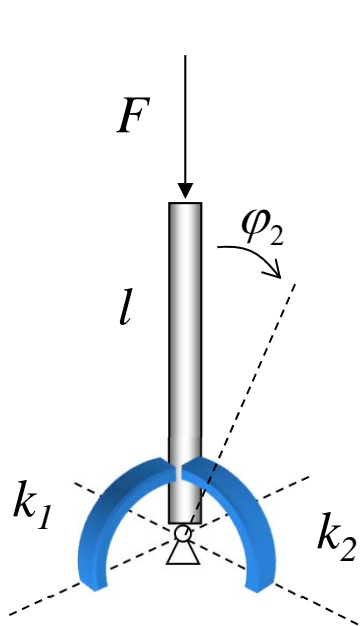
$$\Rightarrow F_{crit} = 4.75$$

Bar example: nature of stationary points

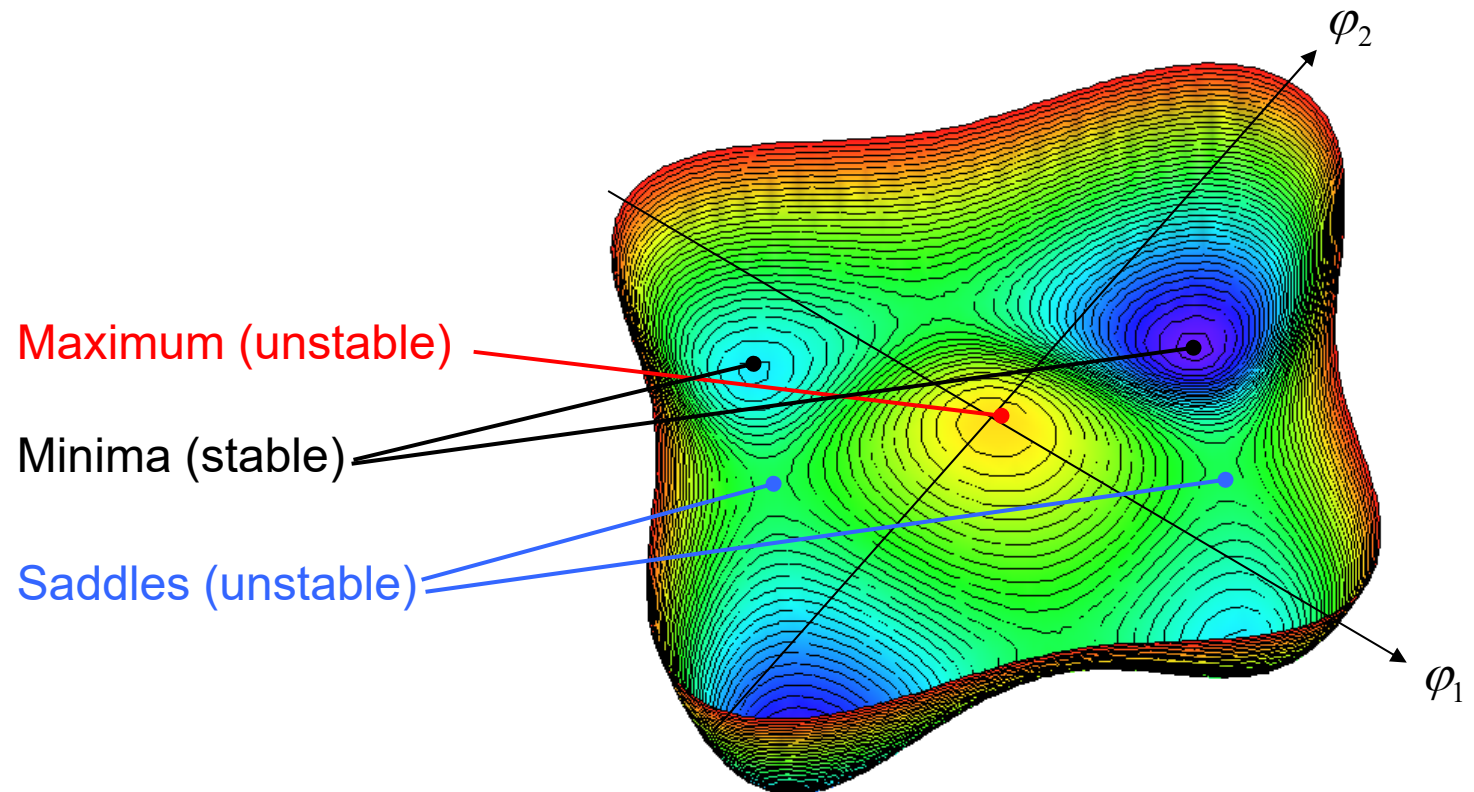


Bar example: nature of stationary points (2)

- Nature of stationary points at $F = 6$:



$$k_1 = 10, k_2 = 9.5, l = 2$$



Contents

- Outline of remaining lectures
- Unconstrained problems
 - Transformation methods
 - Existence of solutions, optimality conditions
 - Nature of stationary points
 - Global optimality

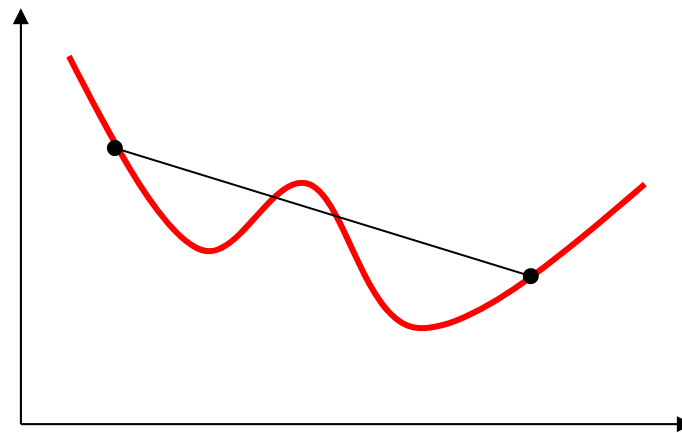
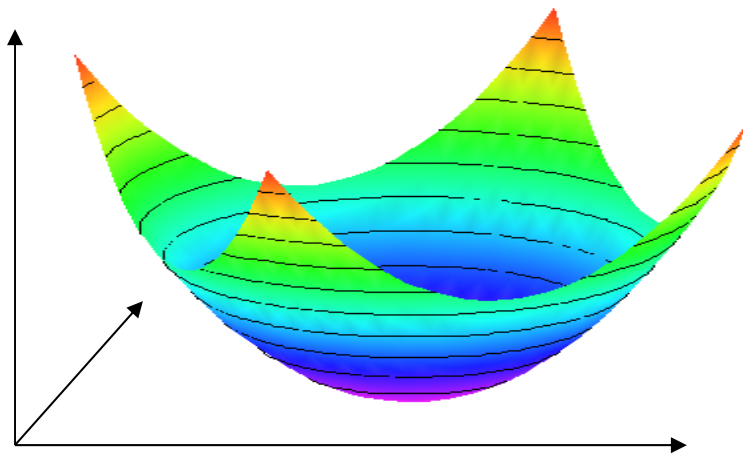
Global optimality



- Optimality conditions for unconstrained problem:
 - First order necessity: $\nabla f(\mathbf{x}^*) = 0$ (stationary point)
 - Second order sufficiency: \mathbf{H} positive definite at \mathbf{x}^*
- Optimality conditions only valid locally:
 - $\Rightarrow \mathbf{x}^*$ *local* minimum
- When can we be sure \mathbf{x}^* is a *global* minimum?

Convex functions

- Convex function: *any line connecting any 2 points on the graph lies above it (or on it):*

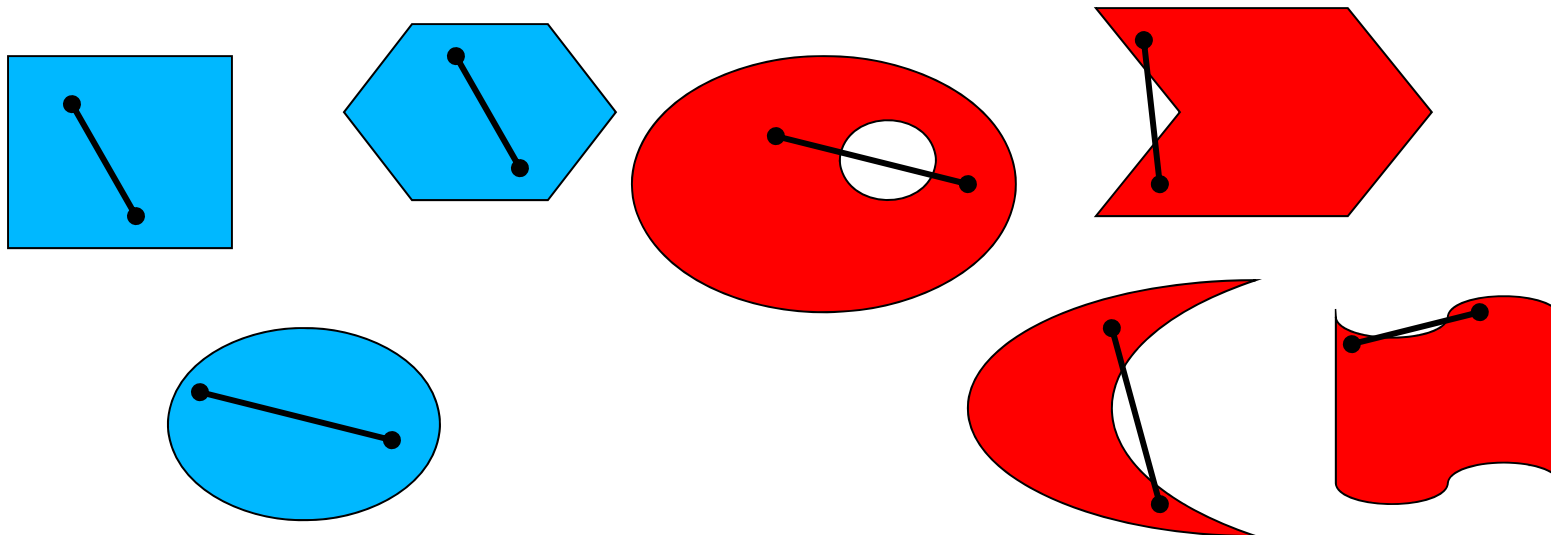


- \mathbf{H} positive (semi-)definite $\Leftrightarrow f$ locally convex
(proof by Taylor approximation)

Convex domains

- Convex set:

“A set S is convex if for every two points x_1, x_2 in S , the connecting line also lies completely inside S ”



Convexity and global optimality (constrained or unconstrained)

If:

- **Objective $f = (\textit{strictly})$ convex function**
- **Feasible domain = convex set** (Ok for unconstrained optimization)



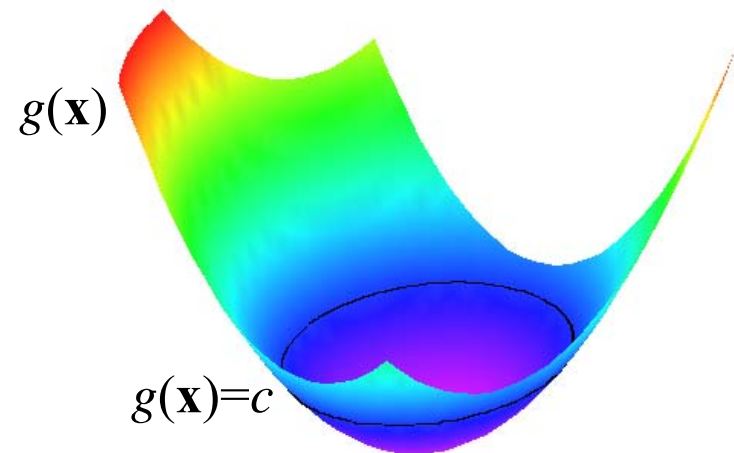
Stationary point = (unique) global minimum

- Special case: f, g, h all linear \Rightarrow *linear programming*
- More general class: *convex optimization*

Convex set properties

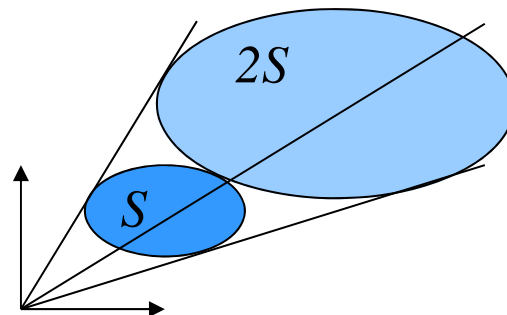
- Level sets (isocontours) of convex functions are convex sets:

$$S = \{\mathbf{x} \mid g(\mathbf{x}) \leq c\}$$



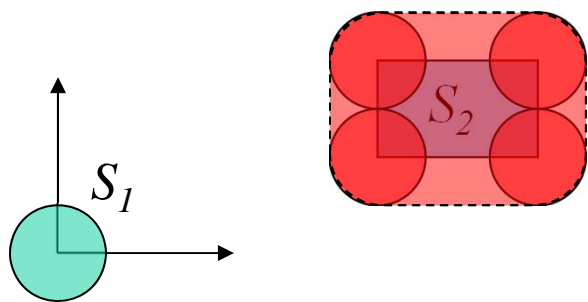
- Scaling:

$$S \text{ convex} \Rightarrow \alpha S \text{ convex}$$



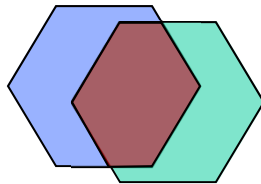
Convex set properties (2)

- Summation: S_1, S_2 convex $\Rightarrow S_1 + S_2$ convex



$$S_1 + S_2 = \{\mathbf{y} \mid \mathbf{y} = \mathbf{x}_1 + \mathbf{x}_2, \mathbf{x}_1 \in S_1, \mathbf{x}_2 \in S_2\}$$

- Intersection: S_1, S_2 convex $\Rightarrow S_1 \cap S_2$ convex



*Applies to feasible domain
defined by multiple constraints*

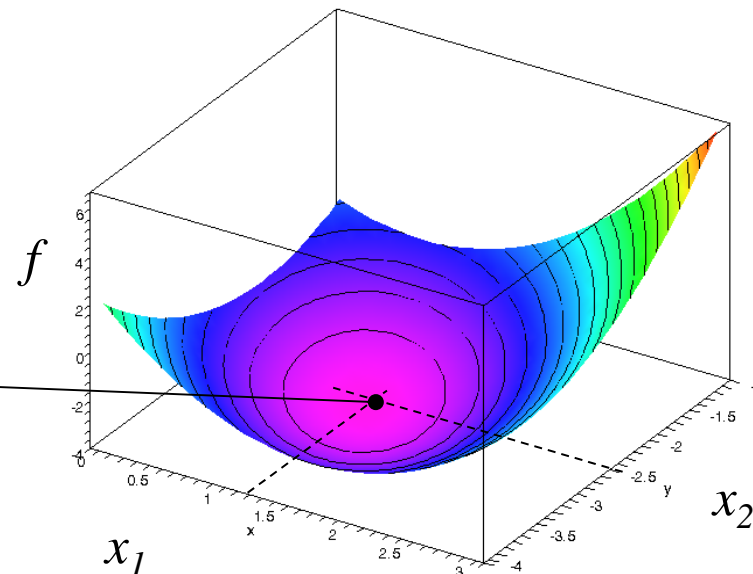
- Union generally nonconvex!

Example

- Quadratic functions with \mathbf{A} positive definite are strictly convex:

$$f(\mathbf{x}) = \frac{1}{2} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix}^T \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} + \begin{Bmatrix} -1 \\ 4 \end{Bmatrix}^T \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} + 2$$

\Rightarrow Stationary point
(1.2, -2.6) must be
*unique global
optimum*



Summary optimality conditions

- Conditions for *local* minimum of unconstrained problem:

- First Order Necessity Condition: $\nabla f = \mathbf{0}$
- Second Order Sufficiency Condition: \mathbf{H} positive definite

- For *convex* f in *convex* feasible domain:
condition for *global* minimum:
 - Sufficiency Condition: $\nabla f = \mathbf{0}$

Summary (2)

- More information: Papalambros 4.1 – 4.4
- Next lecture: **methods** for unconstrained optimization for **single-variable problems**


Sunday May 10: project proposals!



Project proposal [~ 1 A4]

- Context, what is the problem
- Optimization problem formulation (equations not needed):
 - Objective
 - Constraints
 - Design variables (≥ 2): continuous?
- Modeling: how to compute responses?
Which approximations to make?
What model do you already have?
- Cases, variations

Project ideas:
see handouts
Lecture 3

Project info:
see  (Course info +
Assessment – Report
Guidelines)