Introduction to Optimization

Computer Graphics
CMU 15-462/15-662

Last time: physically-based animation

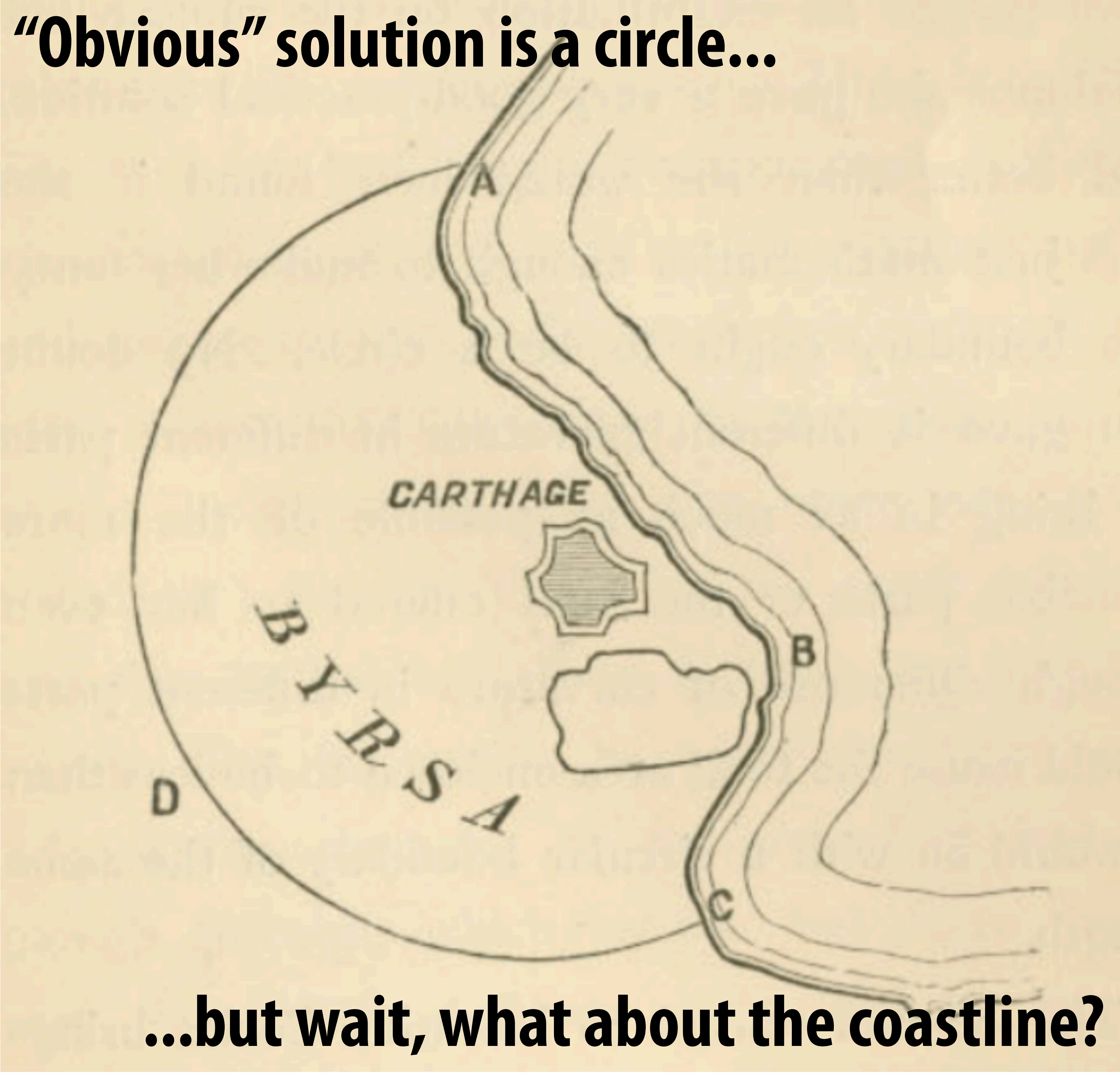
- Use dynamics to drive motion
- Complexity from simple models
- Technique: numerical integration
  - formulate equations of motion
  - take little steps forward in time
  - general, powerful tool
- Today: numerical optimization
  - another general, powerful tool
  - basic idea: “ski downhill” to get a better solution
  - used everywhere in graphics (not just animation)
  - image processing, geometry, rendering, ...

What is an optimization problem?

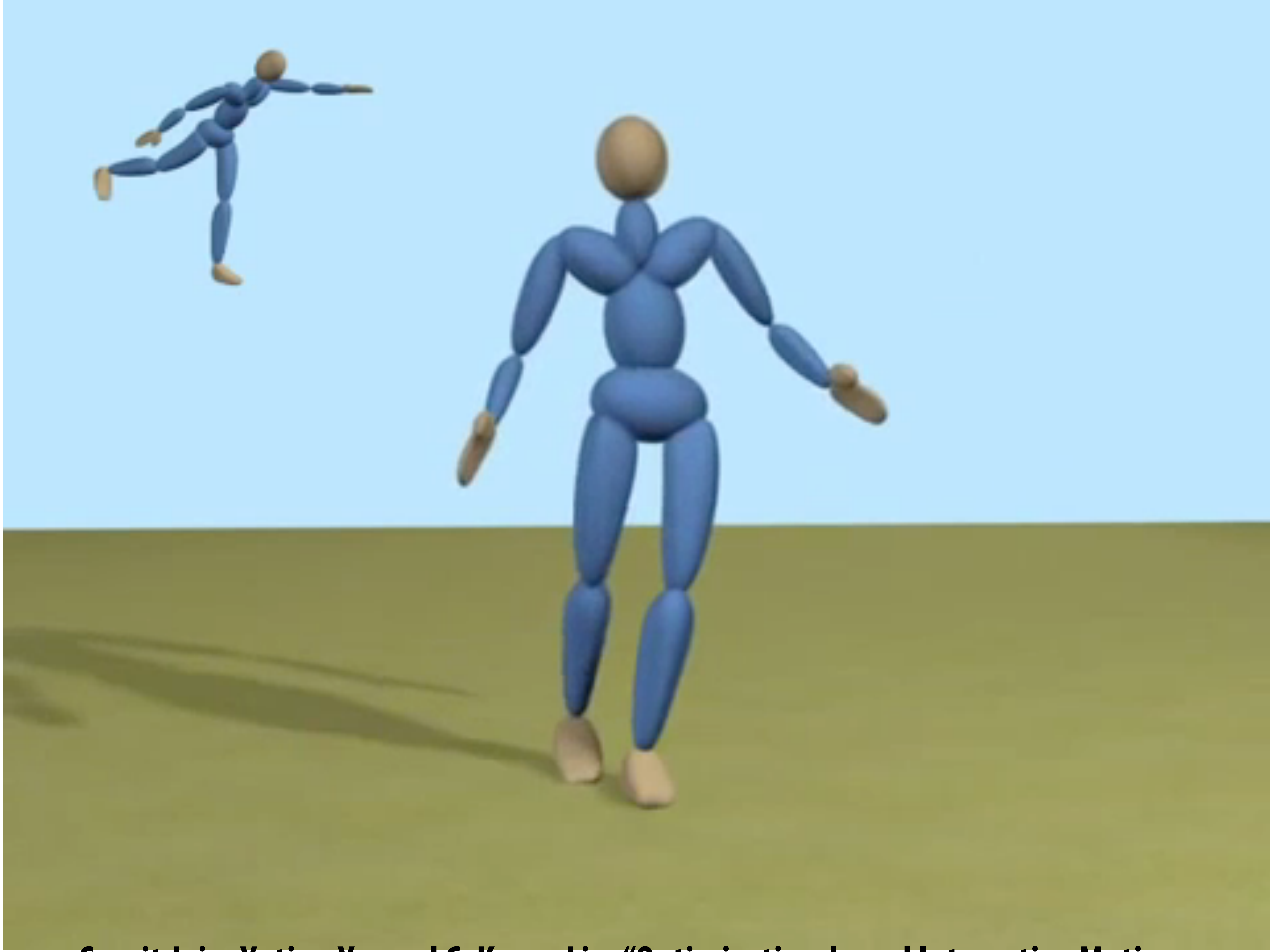
- **Natural human desire: find the best solution among all possibilities (subject to certain constraints)**
- **E.g., cheapest flight, shortest route, tastiest restaurant ...**
- **Has been studied since antiquity, e.g., isoperimetric problem:**

"The first optimization problem known in history was practically solved by Dido, a clever Phoenician princess, who left her Tyrian home and emigrated to North Africa, with all her property and a large retinue, because her brother Pygmalion murdered her rich uncle and husband Acerbas, and plotted to defraud her of the money which he left. On landing in a bay about the middle of the north coast of Africa she obtained a grant from Hiarbas, the native chief of the district, of as much land as she could enclose with an ox-hide. She cut the ox-hide into an exceedingly long strip, and succeeded in enclosing between it and the sea a very valuable territory on which she build Carthage."

—Lord Kelvin, 1893



Optimization in Graphics

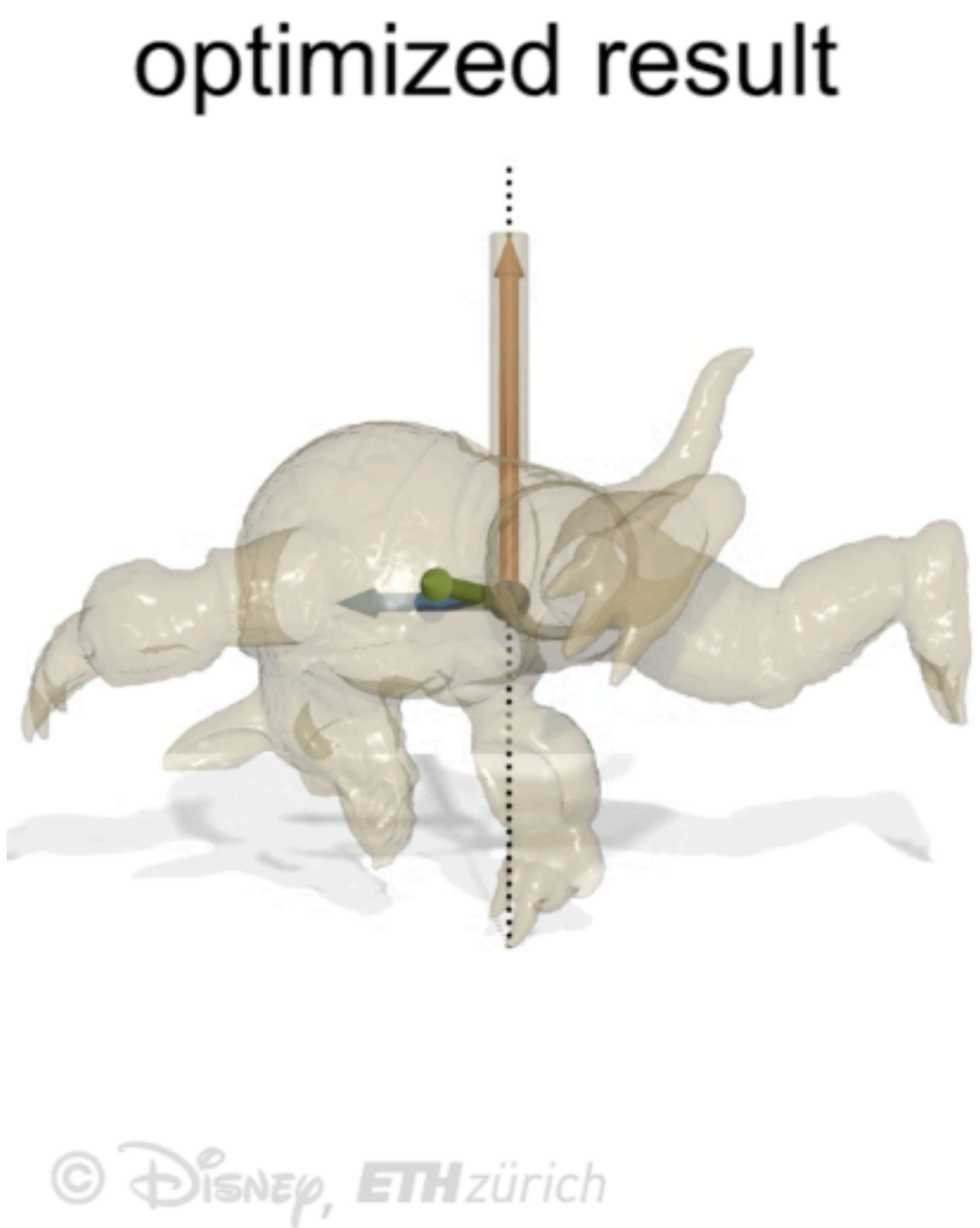


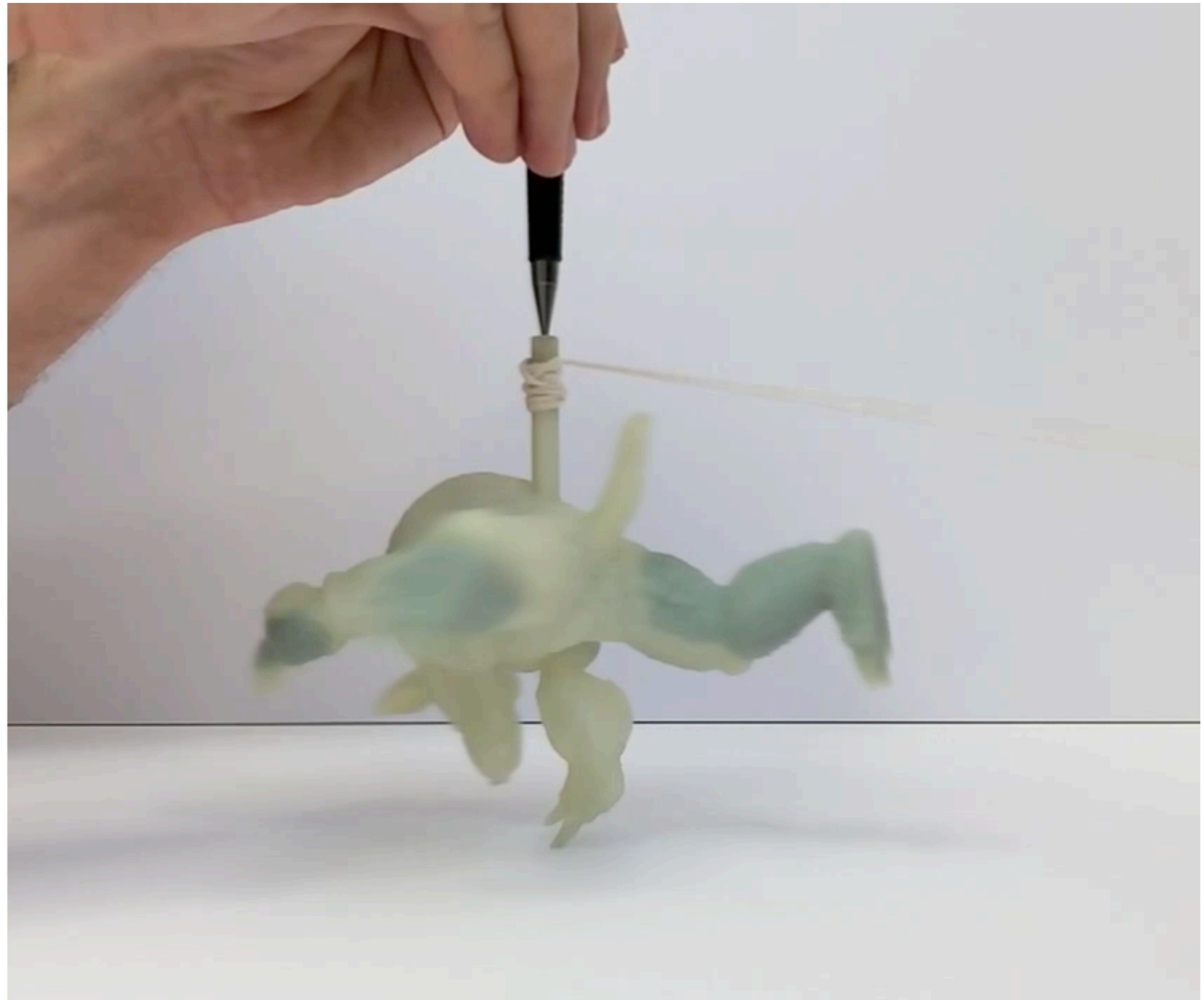
Sumit Jain, Yuting Ye, and C. Karen Liu, “Optimization-based Interactive Motion Synthesis”

Optimization in Graphics

Niloy J. Mitra, Leonidas Guibas, Mark Pauly, "Symmetrization"

Optimization in Graphics





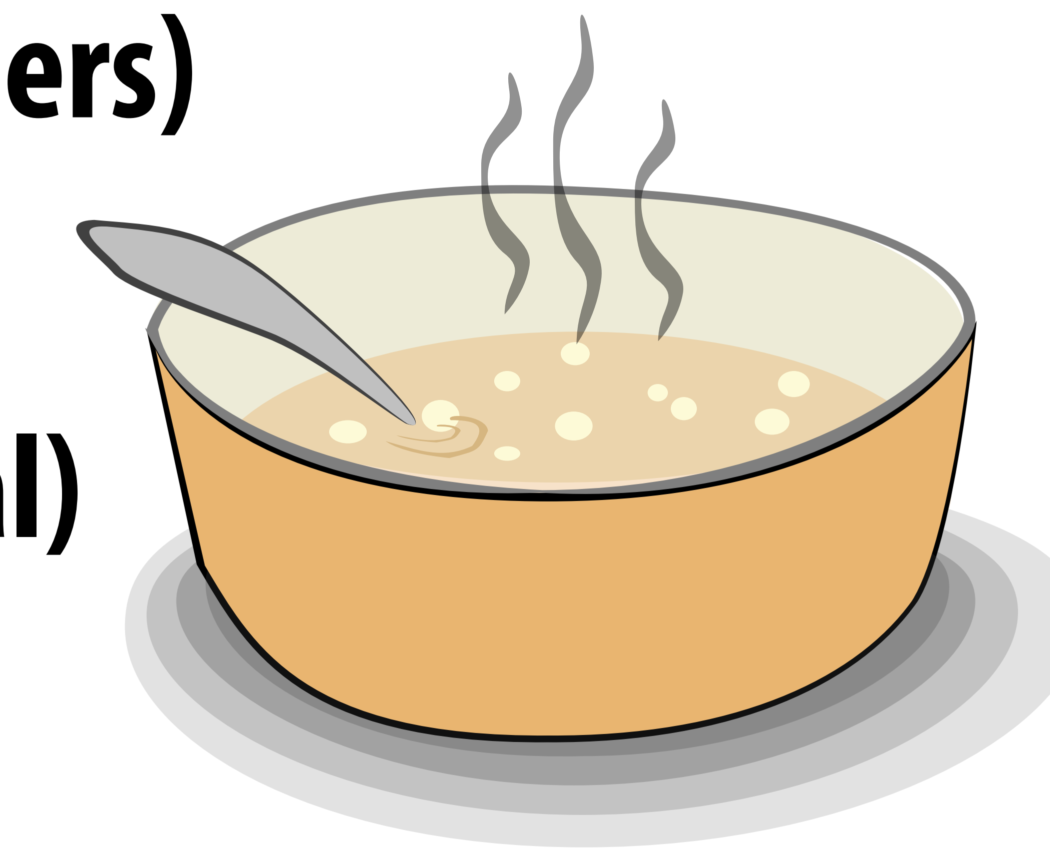
Moritz Bächer, Emily Whiting, Bernd Bickel, Olga Sorkine-Hornung,
"Spin-It: Optimizing Moment of Inertia for Spinnable Objects"

Optimization in Graphics

Nobuyuki Umetani, Yuki Koyama, Ryan Schmidt & Takeo Igarashi,
"Pteromys: Interactive Design and Optimization of Free-formed Free-flight Model Airplanes"

Continuous vs. Discrete Optimization

- **DISCRETE:**
  - domain is a discrete set (e.g., finite or integers)
  - Example: best vegetable to put in a stew
    - Basic strategy? Try them all! (exponential)
    - sometimes clever strategy (e.g., MST)
    - more often, NP-hard (e.g., TSP)



- **CONTINUOUS:**
  - domain is not discrete (e.g., real numbers)
  - Example: best temperature to cook an egg
  - still many (NP-)hard problems, but also large classes of "easy" problems (e.g., convex)

Optimization Problem in Standard Form

- **Can formulate most continuous optimization problems this way:**

"objective": how much does solution x cost?

$(f_i : \mathbb{R}^n \to \mathbb{R},\ i = 0, \dots, m)$

often (but not always) continuous, differentiable, ...

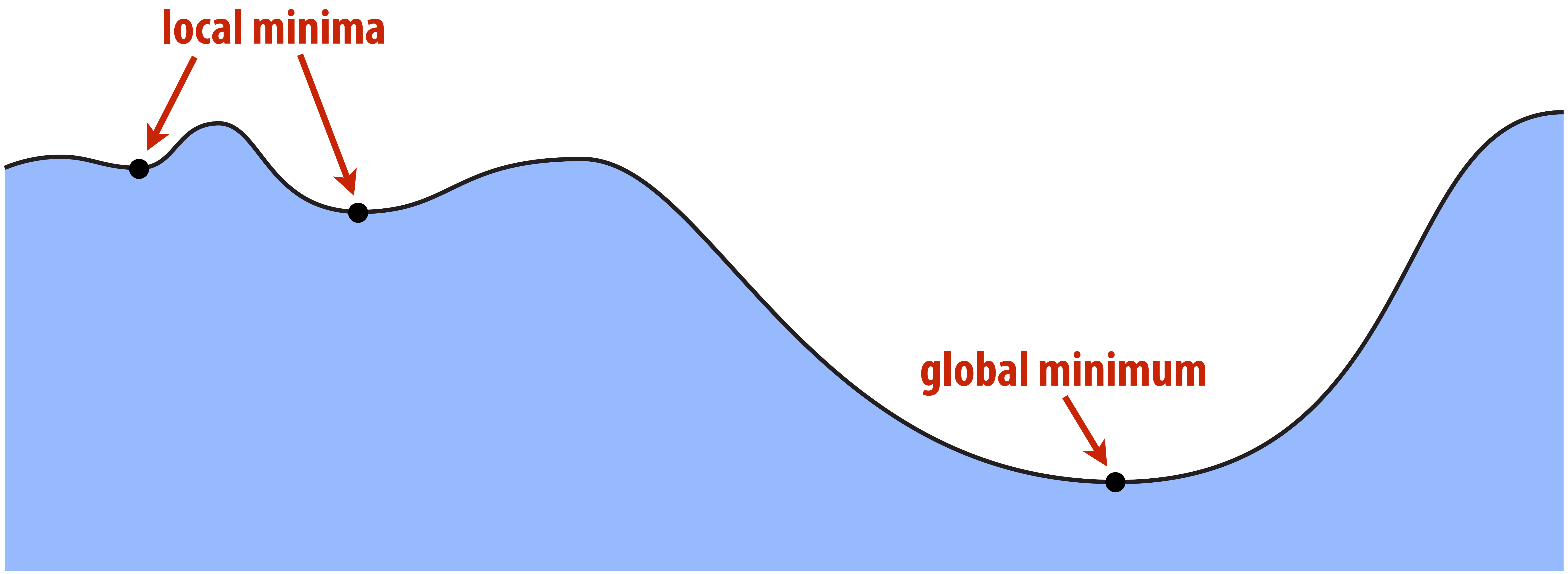
$$\min_{x \in \mathbb{R}^n} \quad f_0(x)$$
$$\text{subject to} \quad f_i(x) \leq b_i,\ i = 1, \dots, m$$

"constraints": what must be true about x? ("x is feasible")

- **Optimal solution x* has smallest value of f_0 among all feasible x**
- **Q: What if we want to maximize something instead?**
- **A: Just flip the sign of the objective!**
- **Q: What if we want equality constraints, rather than inequalities?**
- **A: Include two constraints: g(x) ≤ c and g(x) ≤ -c**

Local vs. Global Minima

- Global minimum is absolute best among all possibilities
- Local minimum is best “among immediate neighbors”

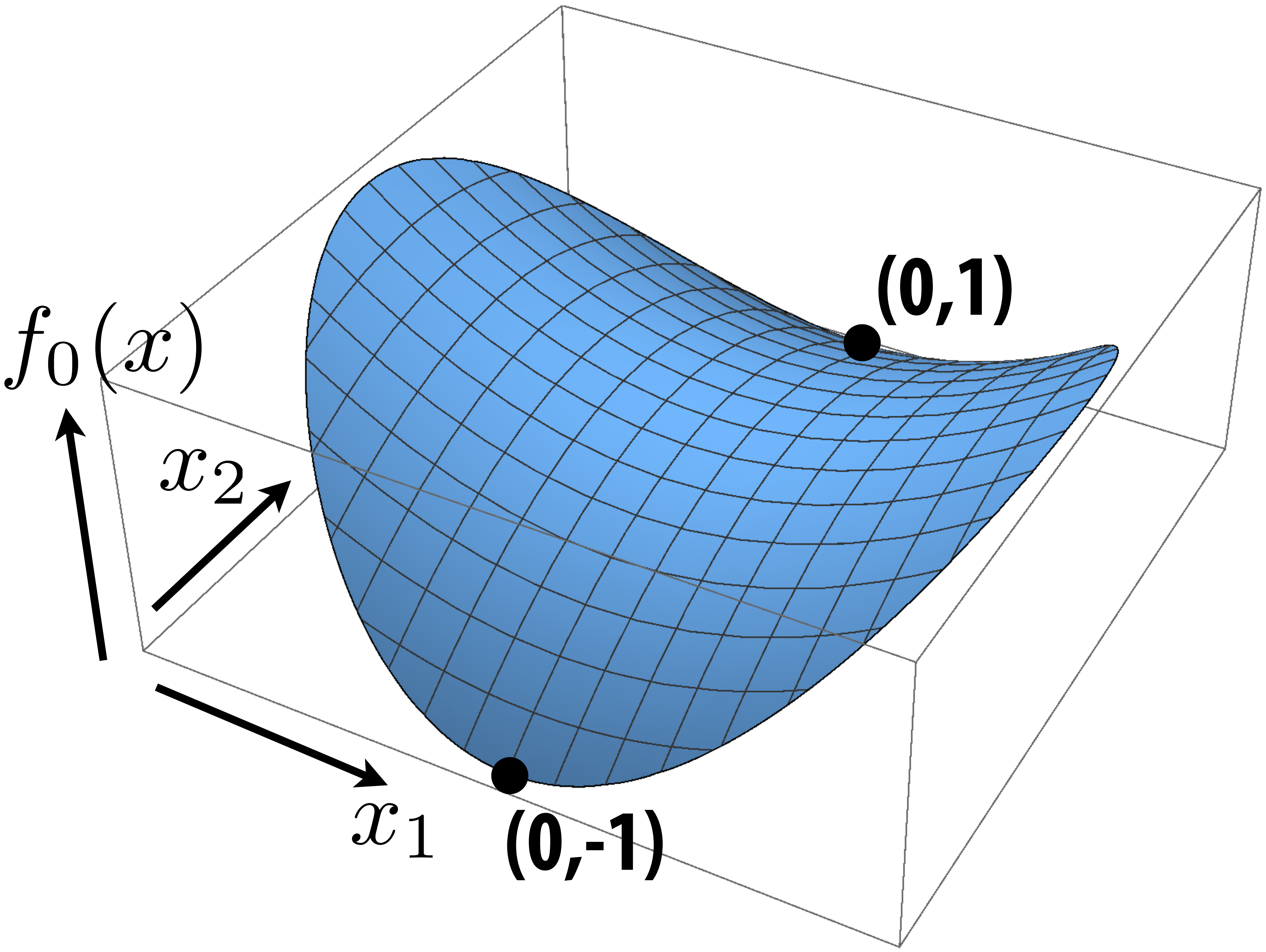


Philosophical question: does a local minimum “solve” the problem?

Depends on the problem! (E.g., real protein folding is local minimum)

Other times, local minima can be really bad (e.g., path planning)

Optimization Problem, Visualized



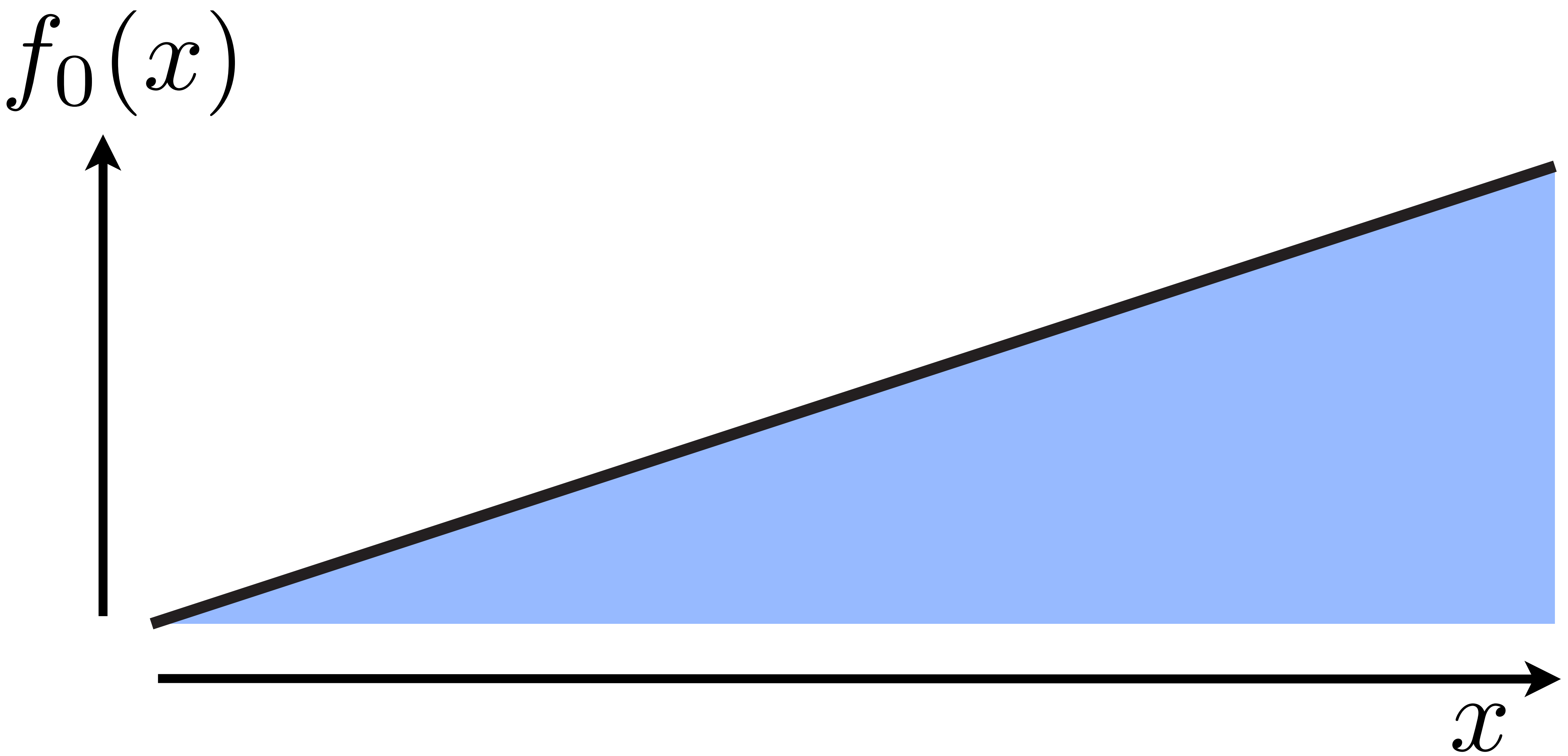
$$\min_{x \in \mathbb{R}^2} \quad x_1^2 - x_2^2$$
$$\text{s.t.} \quad x_1^2 + x_2^2 - 1 \leq 0$$

Q: Is this an optimization problem in standard form? **A: Yes.**

Q: Where is the optimal solution? **A: There are two, (0,1), (0,-1).**

Existence & Uniqueness of Minimizers

- Already saw that (global) minimizer is not unique.
- Does it always exist? Why?
- Just consider all possibilities and take the smallest one, right?



perfectly reasonable optimization problem

$$\min_{x \in \mathbb{R}} x$$

clearly has no solution (can always pick smaller x)

- WRONG! Not all objectives are bounded from below.
- It's like that old adage: "no matter how good you are, there will always be someone better than you."

Feasibility

- Ok, but suppose the objective is bounded from below.
- Then we can just take the best feasible solution, right?

value of objective doesn't depend on x;
all feasible solutions are equally good

$$\min_{x \in \mathbb{R}^n} \quad 0$$
$$\text{subject to} \quad f_i(x) \leq b_i, \; i = 1, \ldots, m$$

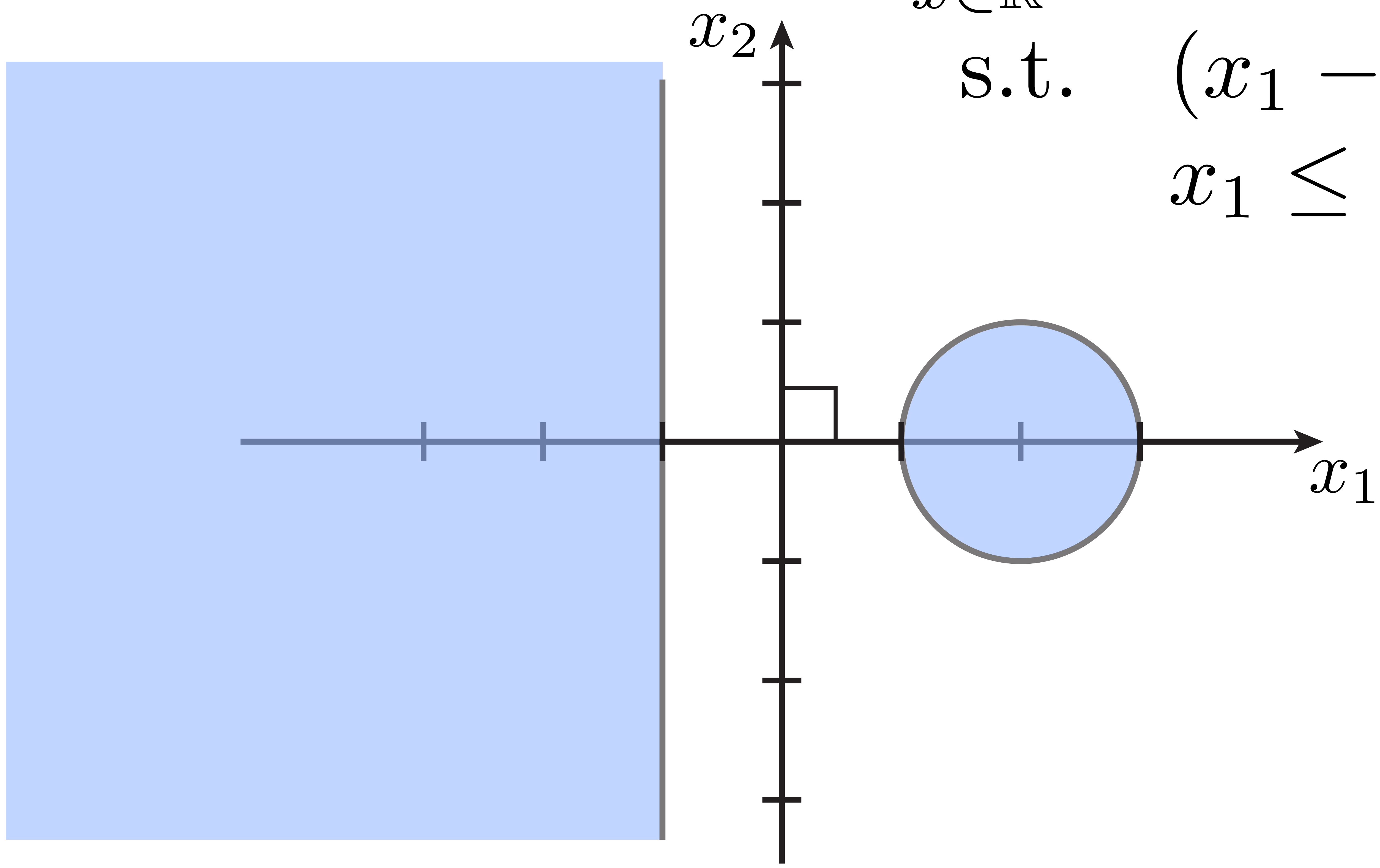
problem now is just finding a feasible solution—
which can be really hard (or impossible!)

- Not if there aren't any!
- Every system of equations is an optimization problem.
- But not all problems have solutions!
- (You'll appreciate this more as you get older.)

Feasibility - Example

Q: Is this problem feasible?

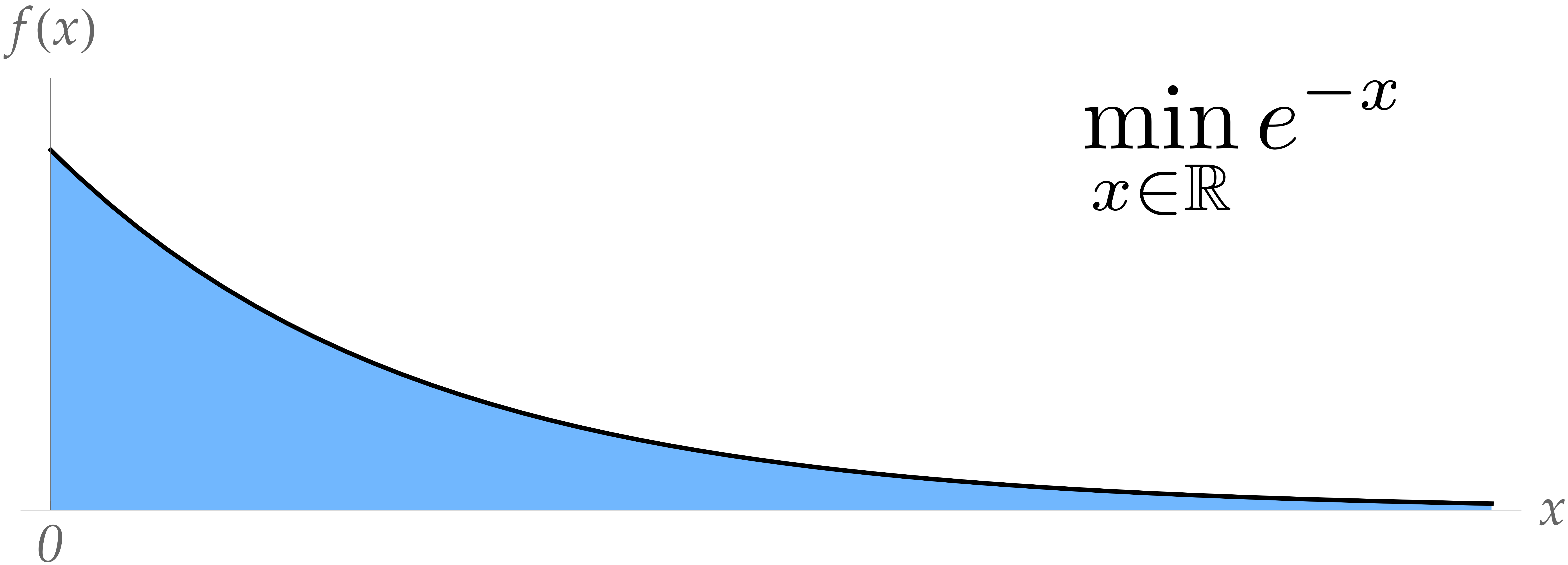
$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & \sin(x_1) + x_2^2 \\ \text{s.t.} \quad & (x_1 - 2)^2 + x_2^2 \leq 1, \\ & x_1 \leq -1 \end{aligned}$$



A: No—the two sublevel sets (points where f_i(x) ≤ 0) have no common points, i.e., they do not overlap.

Existence & Uniqueness of Minimizers, cont.

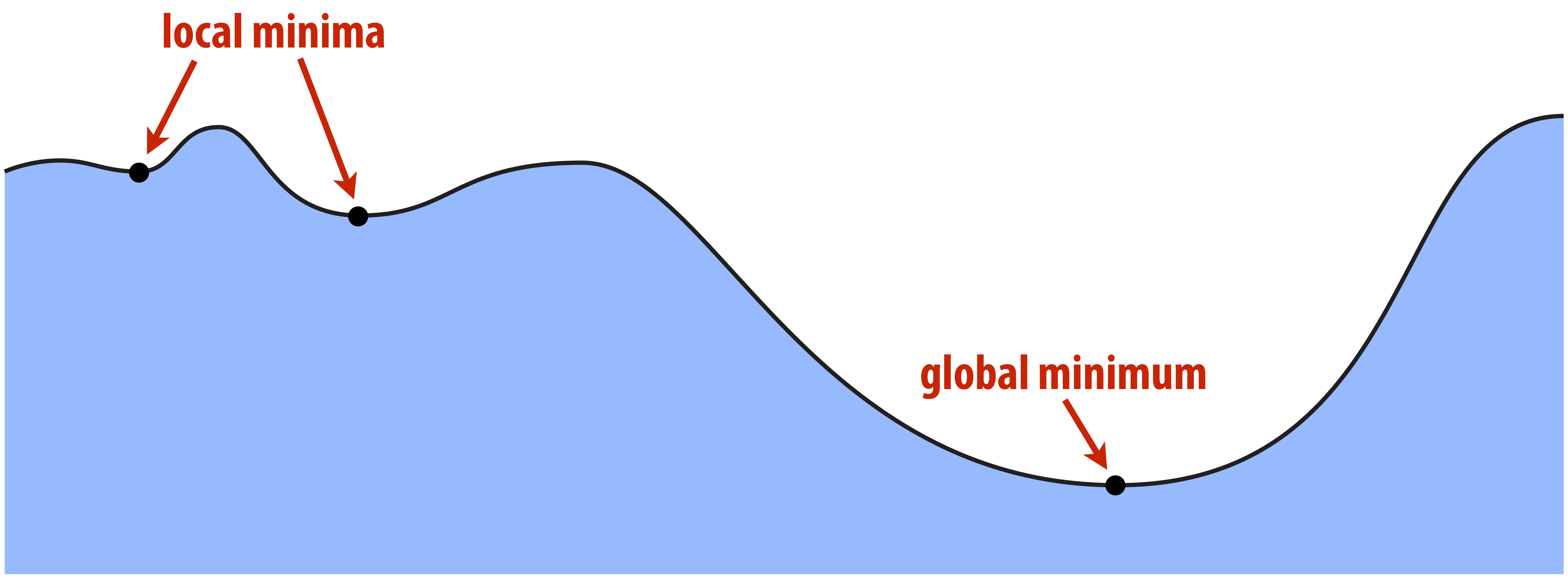
- Even being bounded from below is not enough:



- No matter how big x is, we never achieve the lower bound (0)
- So when does a solution exist? Two sufficient conditions:
- Extreme value theorem: continuous objective & compact domain
- Coercivity: objective goes to $+\infty$ as we travel (far) in any direction

Characterization of Minimizers

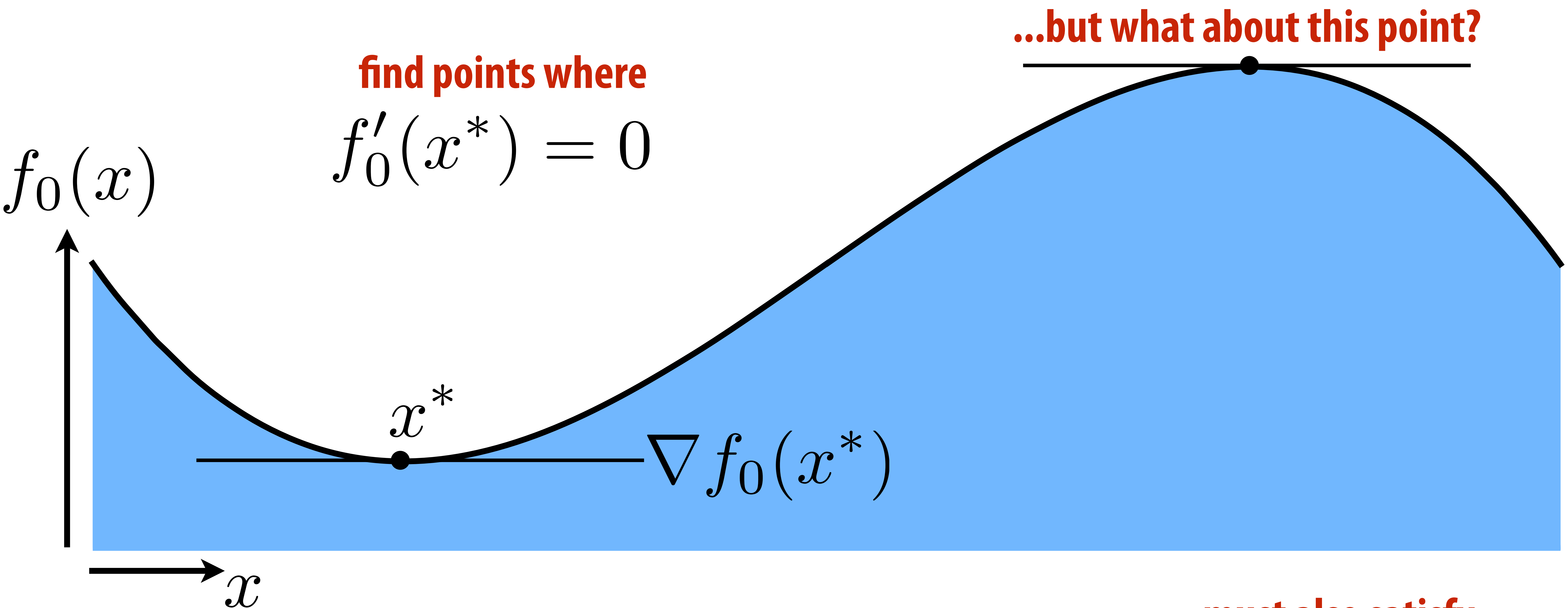
- Ok, so we have some sense of when a minimizer might exist
- But how do we know a given point x is a minimizer?



- Checking if a point is a global minimizer is (generally) hard
- But we can certainly test if a point is a local minimum (ideas?)
- (Note: a global minimum is also a local minimum!)

Characterization of Local Minima

- Consider an objective f_0: R → R. How do you find a minimum?
- (Hint: you may have memorized this formula in high school!)



- Also need to check second derivative (how?)
- Make sure it's positive
- Ok, but what does this all mean for more general functions f_0?

must also satisfy

$$f_0''(x^*) \geq 0$$

Optimality Conditions (Unconstrained)

- In general, our objective is $f_0: R^n \rightarrow R$
- How do we test for a local minimum?
- 1st derivative becomes gradient; 2nd derivative becomes Hessian

$$\nabla f := \begin{bmatrix} \partial f / \partial x_1 \\ \vdots \\ \partial f / \partial x_n \end{bmatrix}$$

GRADIENT
(measures "slope")

$$\nabla^2 f := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial f}{\partial x_n^2} \end{bmatrix}$$

HESSIAN
(measures "curvature")

- Optimality conditions?

$$\nabla f_0(x^*) = 0$$

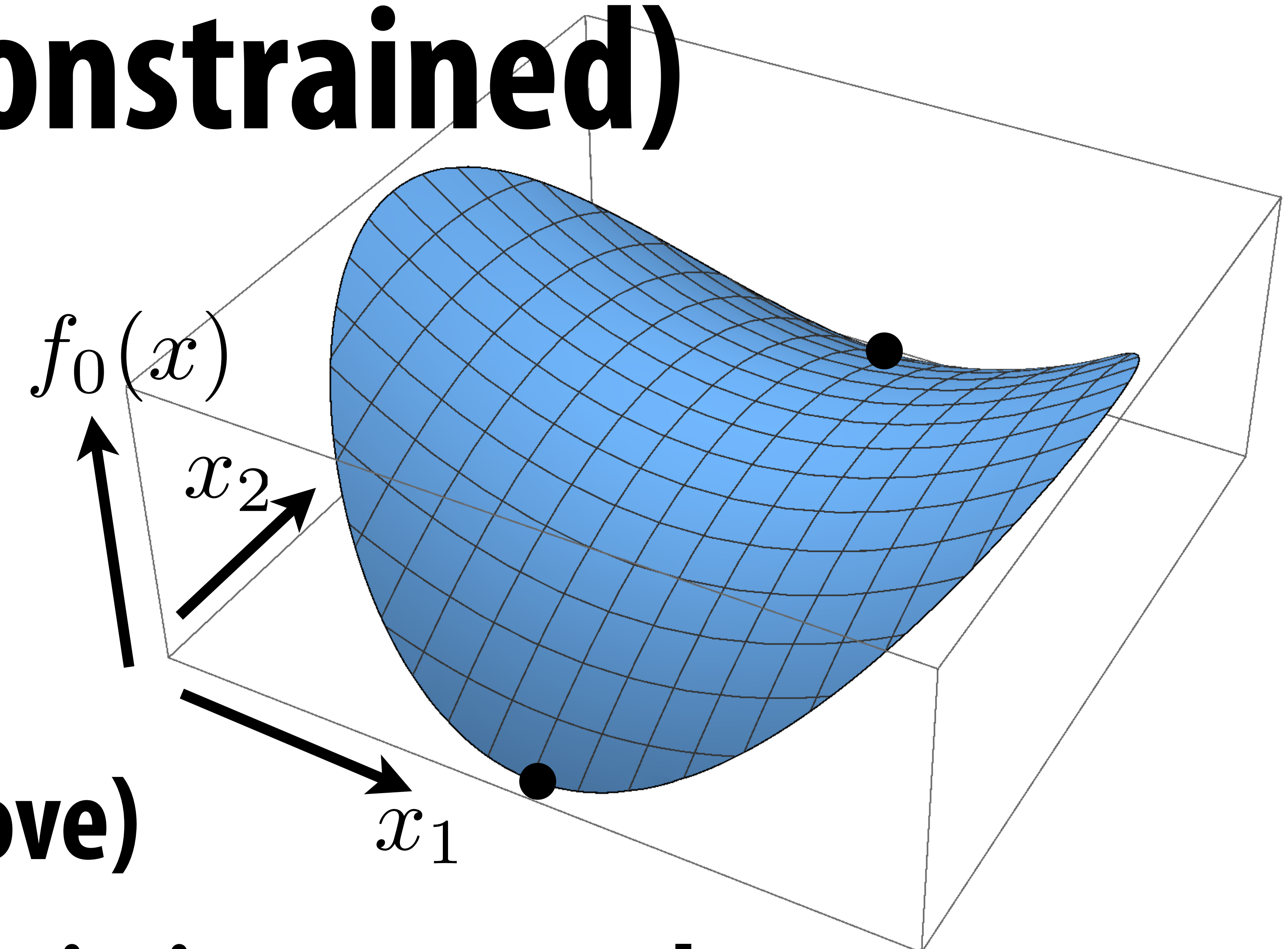
1st order

positive semidefinite (PSD)
($u^TAu \geq 0$ for all u)

$$\nabla^2 f_0(x^*) \succeq 0$$

2nd order

Optimality Conditions (Constrained)



- What if we have constraints?
- Is gradient at minimizer still zero?
- Is Hessian at minimizer still PSD?
- Not necessarily! (See example above)
- In general, any (local or global) minimizer must at least satisfy the Karush–Kuhn–Tucker (KKT) conditions:

$$\exists \lambda_i \text{ s.t.} \quad \nabla f_0(x^*) = -\sum_{i=1}^{n} \lambda_i \nabla f_i(x^*) \qquad \text{stationarity}$$

$$f_i(x^*) \leq 0, \; i = 1, \ldots, n \qquad \text{primal feasibility}$$

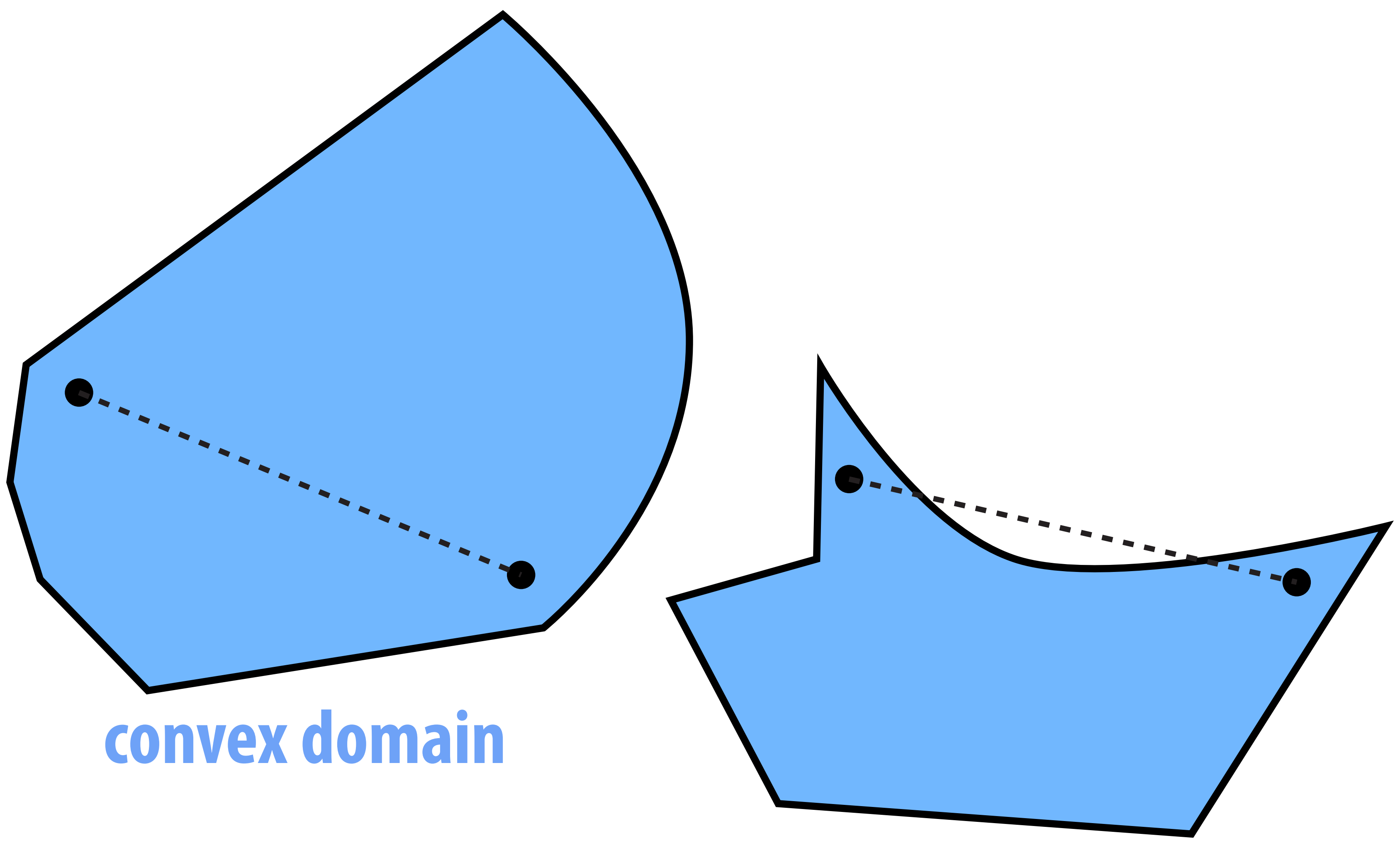
$$\lambda_i \geq 0, i = 1, \ldots, n \qquad \text{dual feasibility}$$

$$\lambda_i f_i(x^*) = 0, \; i = 1, \ldots, n \qquad \text{complementary slackness}$$

- ...we won't work with these in this class!
(But good to know where to look.)

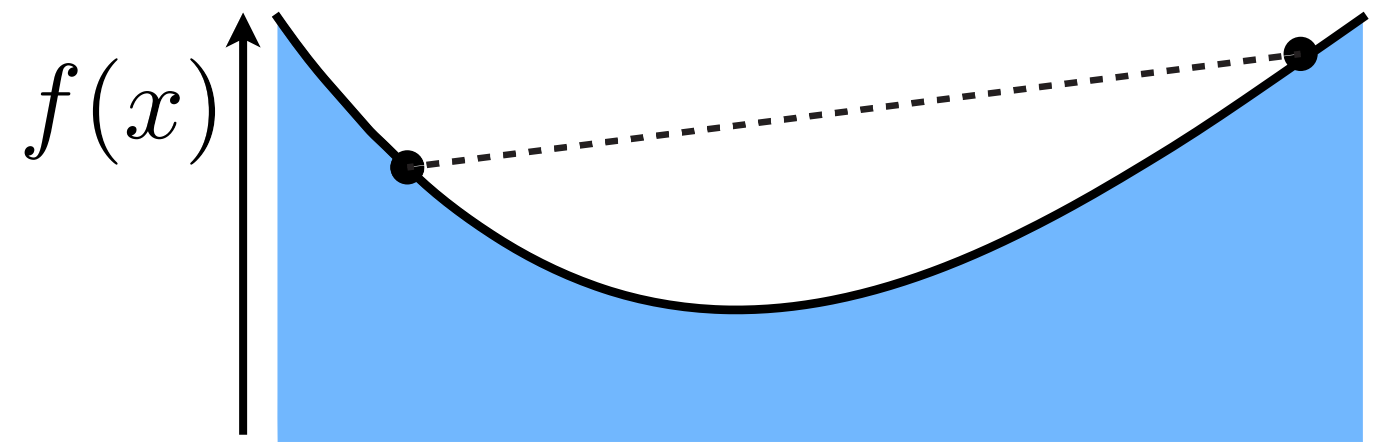
Convex Optimization

- Special class of problems that are almost always "easy" to solve (polynomial-time!)
- Problem convex if it has a convex domain and convex objective

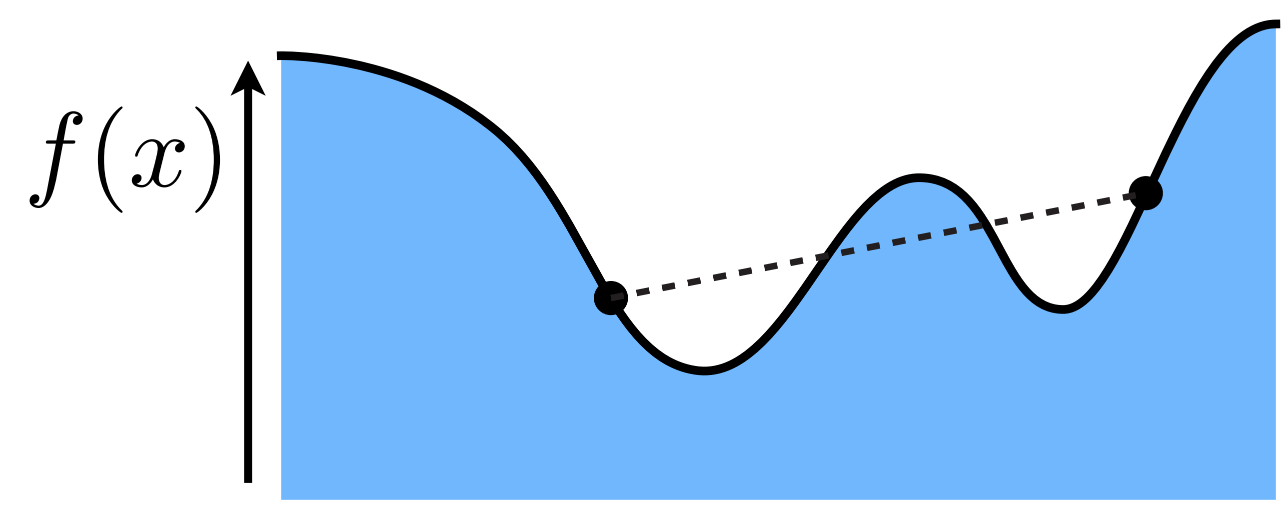


convex domain

noconvex domain



convex objective



nonconvex objective

- Why care about convex problems in graphics?
  - can make guarantees about solution (always the best)
  - doesn't depend on initialization (strong convexity)
  - often quite efficient, but not always

Convex Quadratic Objectives & Linear Systems

- Very important example: convex quadratic objective
- Already saw this with, e.g., quadric error simplification
- Valuable "variational" way of looking at many common equations
- Can be expressed via positive-semidefinite (PSD) matrix:

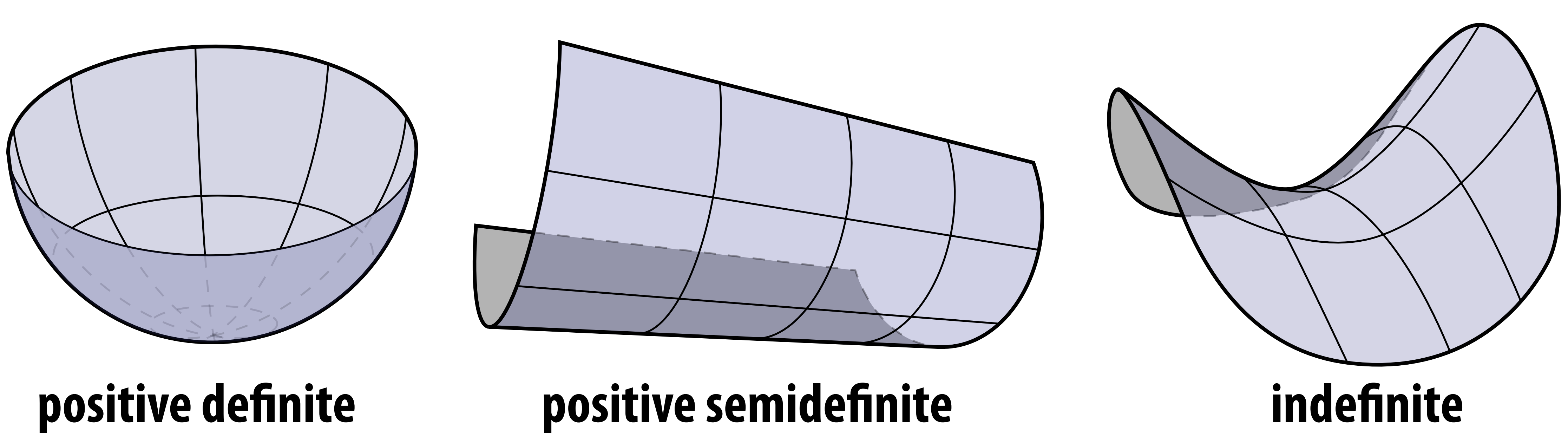
$$f_0(x) = \frac{1}{2}x^TAx - x^Tb, \;\; A \succeq 0$$

just solve a linear system!

- Q: 1st-order optimality condition? $Ax = b$

satisfied by definition

- Q: 2nd-order optimality condition? $A \succeq 0$



Sadly, life is not usually that easy.
How do we solve optimization problems in general?

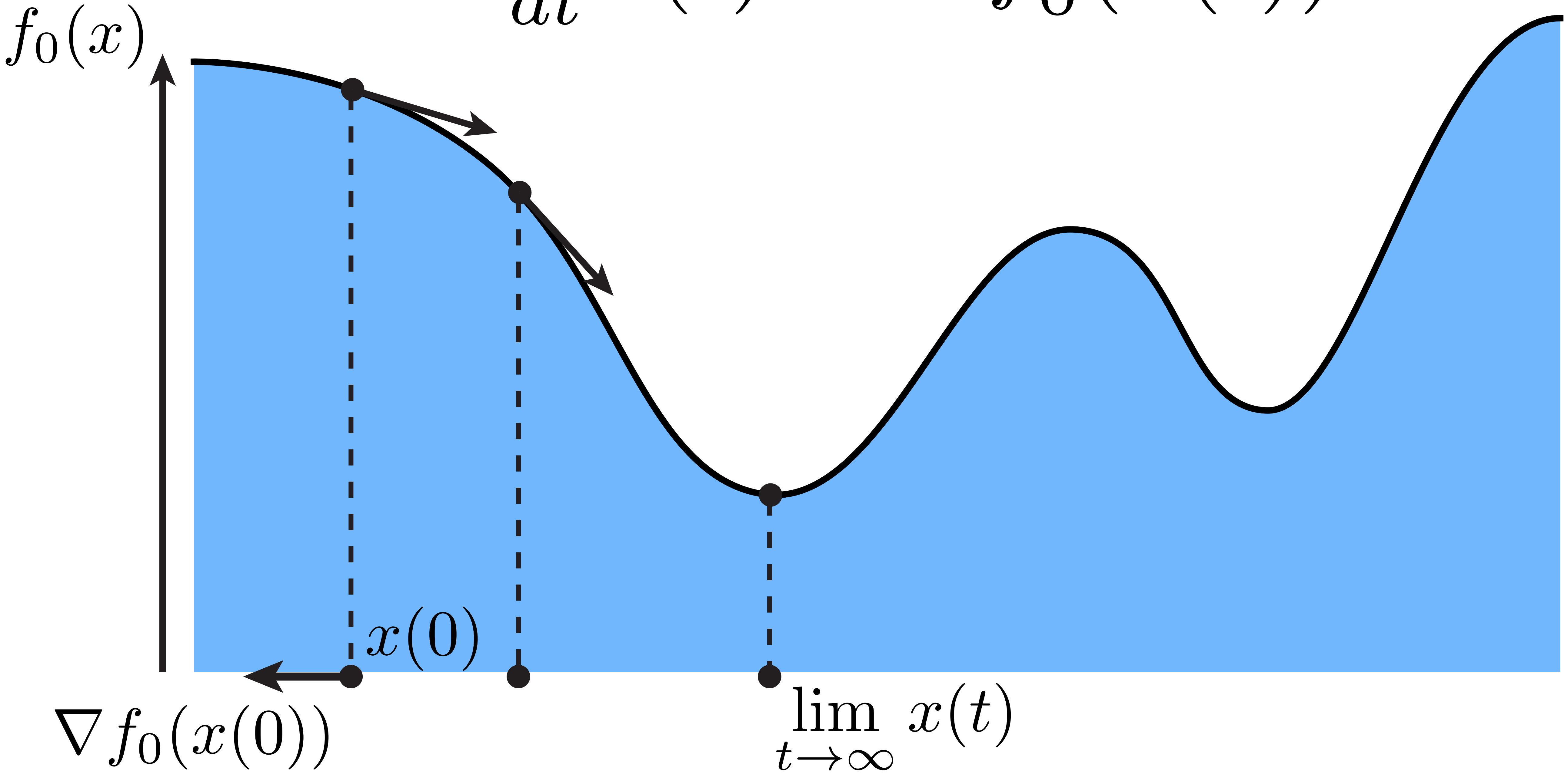
Descent Methods

An idea as old as the hills:

Gradient Descent (1D)

- **Basic idea: follow the gradient "downhill" until it's zero**
- **(Zero gradient was our 1st-order optimality condition)**

$$\frac{d}{dt}x(t) = -f_0'(x(t))$$

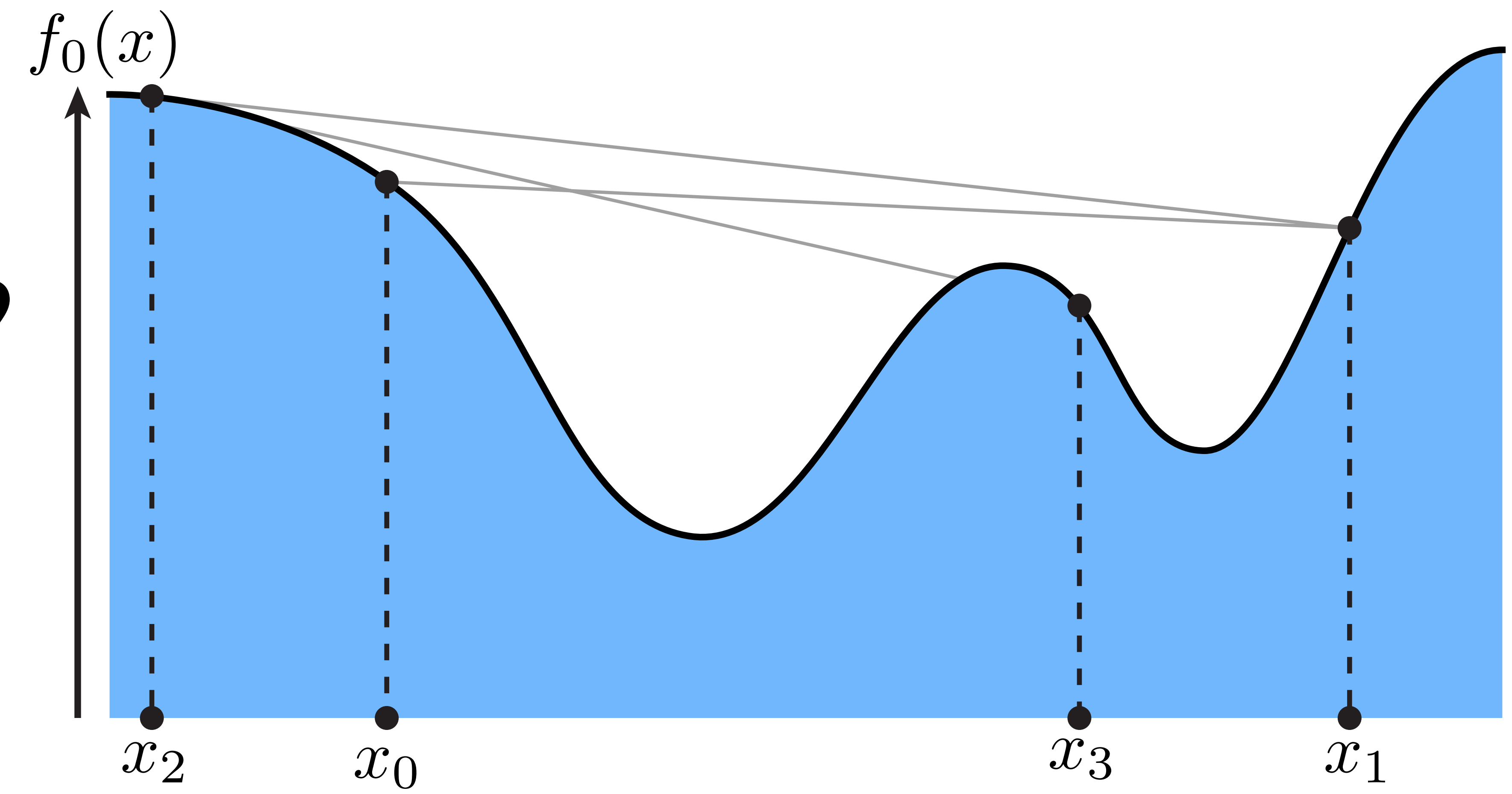


- **Do we always end up at a (global) minimum?**
- **How do we compute gradient descent in practice?**

Gradient Descent Algorithm (1D)

- Did you notice that gradient descent equation is an ODE?
- Q: How do we solve it numerically? $$\frac{d}{dt}x(t) = -f_0'(x(t))$$
- One way: forward Euler:

$$x_{k+1} = x_k - \tau f_0'(x_k)$$



- Q: How do we pick the time step?
- If we're not careful, we'll go zipping all over the place; won't make any progress.
- Basic idea: use "step control" to determine step size based on value of objective & derivatives.
- A careful strategy (e.g., Armijo-Wolfe) can guarantee convergence at least to a local minimum.
- For now we will do something simpler: make τ really small!

Gradient Descent Algorithm (nD)

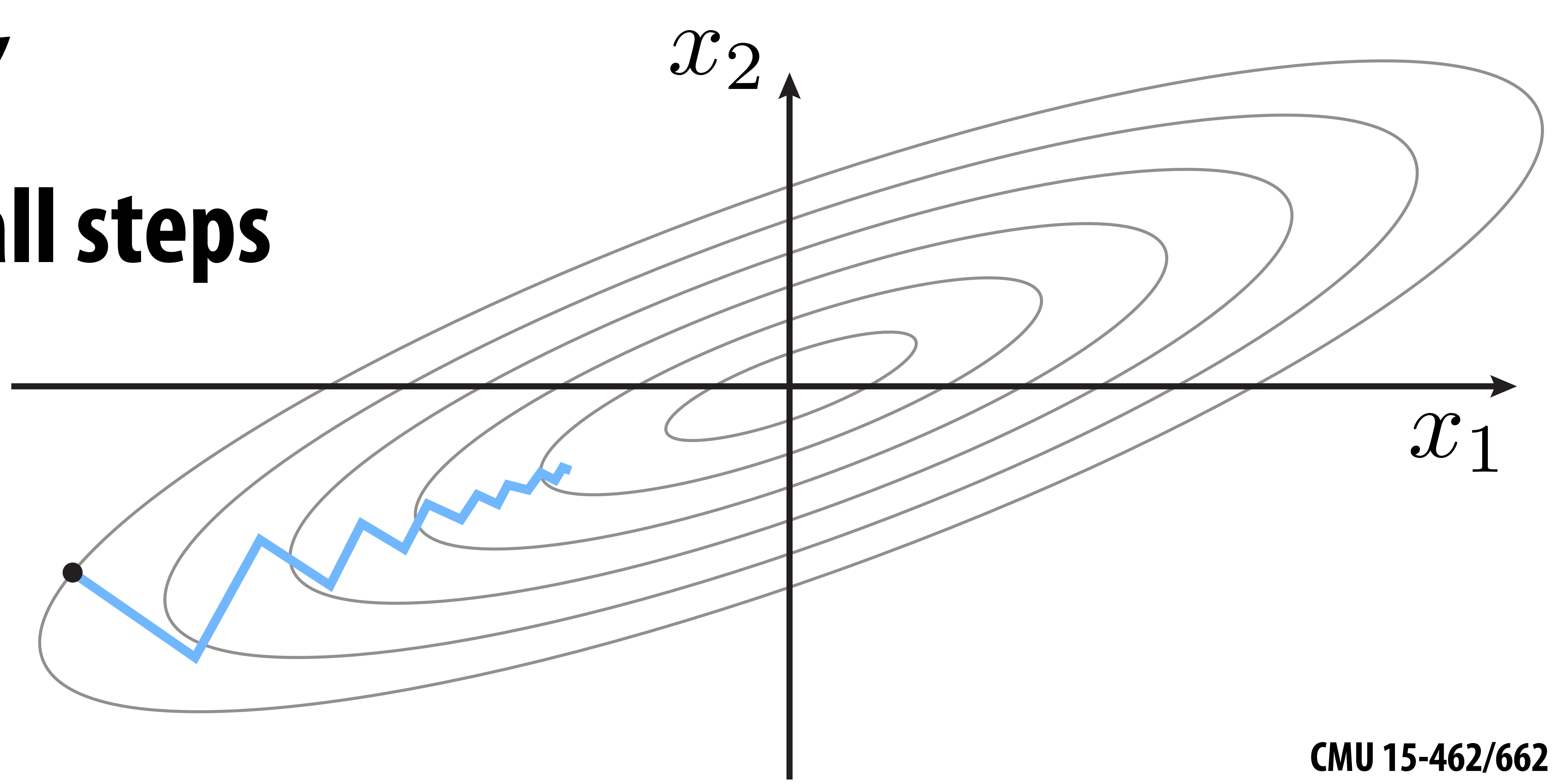
- **Q: How do we write gradient descent equation in general?**

$$\frac{d}{dt}x(t) = -\nabla f_0(x(t))$$

- **Q: What's the corresponding discrete update?**

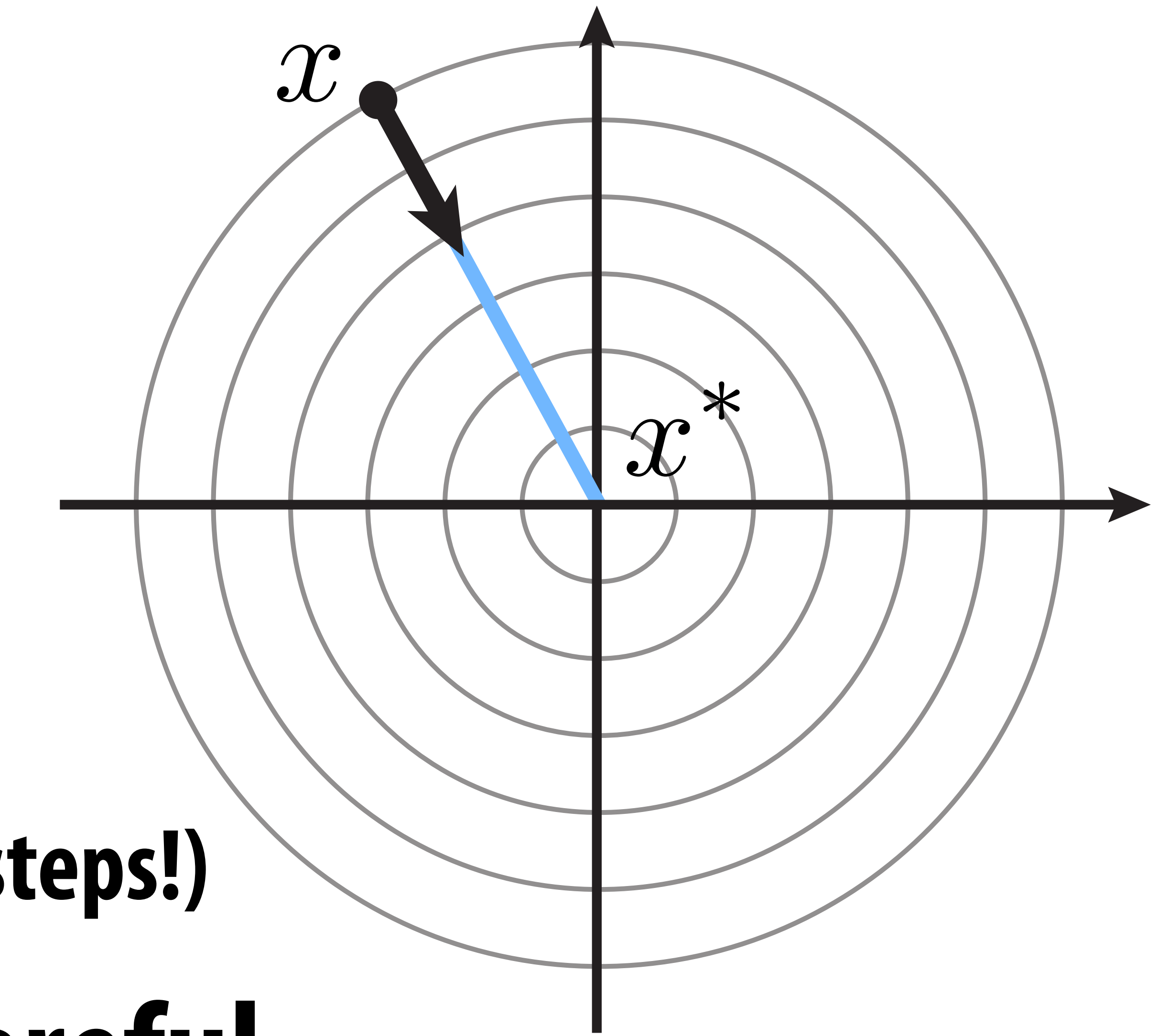
$$x_{k+1} = x_k - \tau \nabla f_0(x_k)$$

- **Basic challenge in nD:**
  - **solution can "oscillate"**
  - **takes many, many small steps**
  - **very slow to converge**



Higher Order Descent

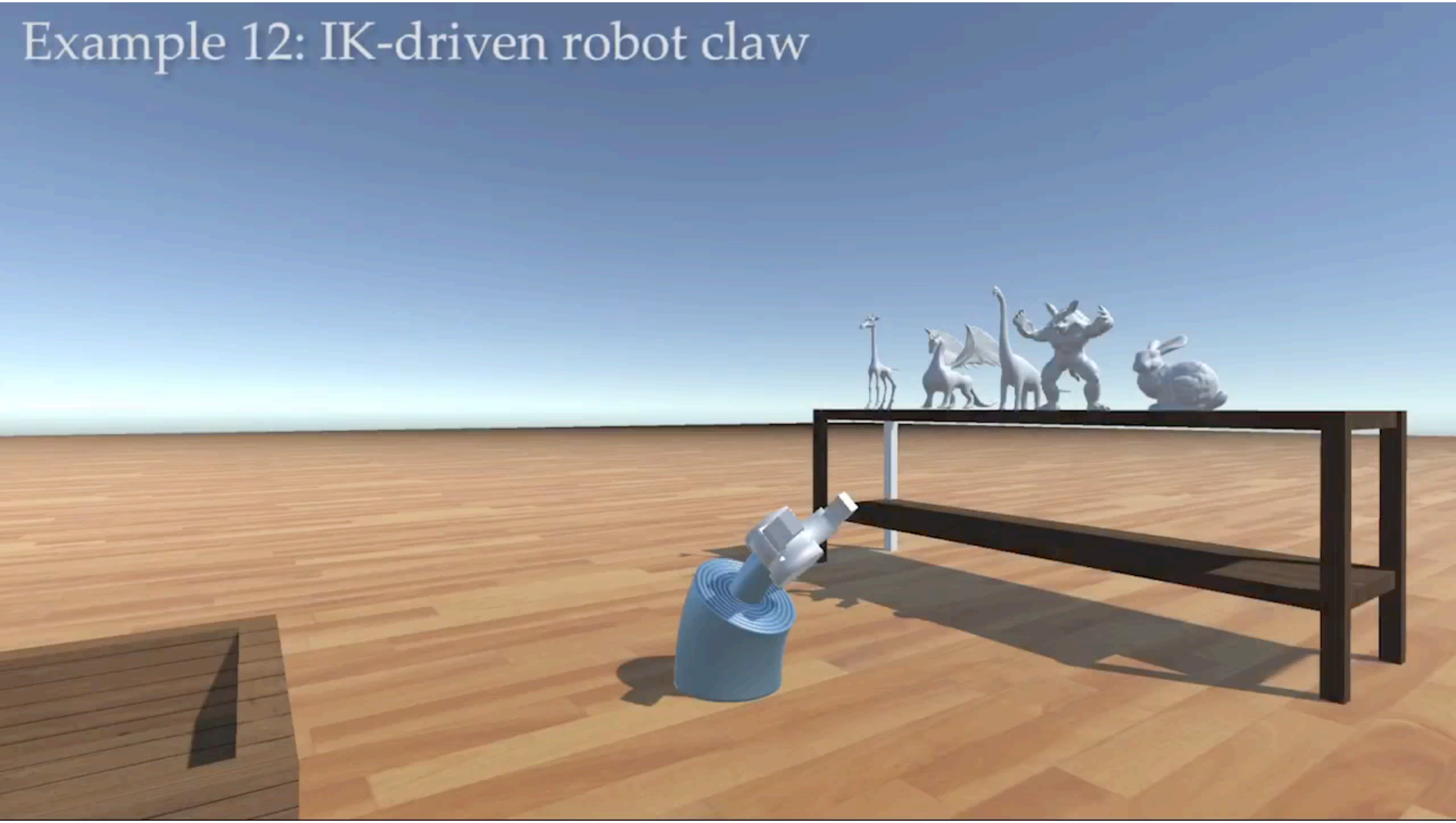
- **General idea: apply a coordinate transformation so that the local energy landscape looks more like a "round bowl"**
- **Gradient now points directly toward nearby minimizer**
- **Most basic strategy: Newton's method:**



$$x_{k+1} = x_k - \tau \underbrace{(\nabla^2 f_0(x_k))^{-1}}_{\text{Hessian inverse}} \overbrace{\nabla f_0(x_k)}^{\text{gradient}}$$

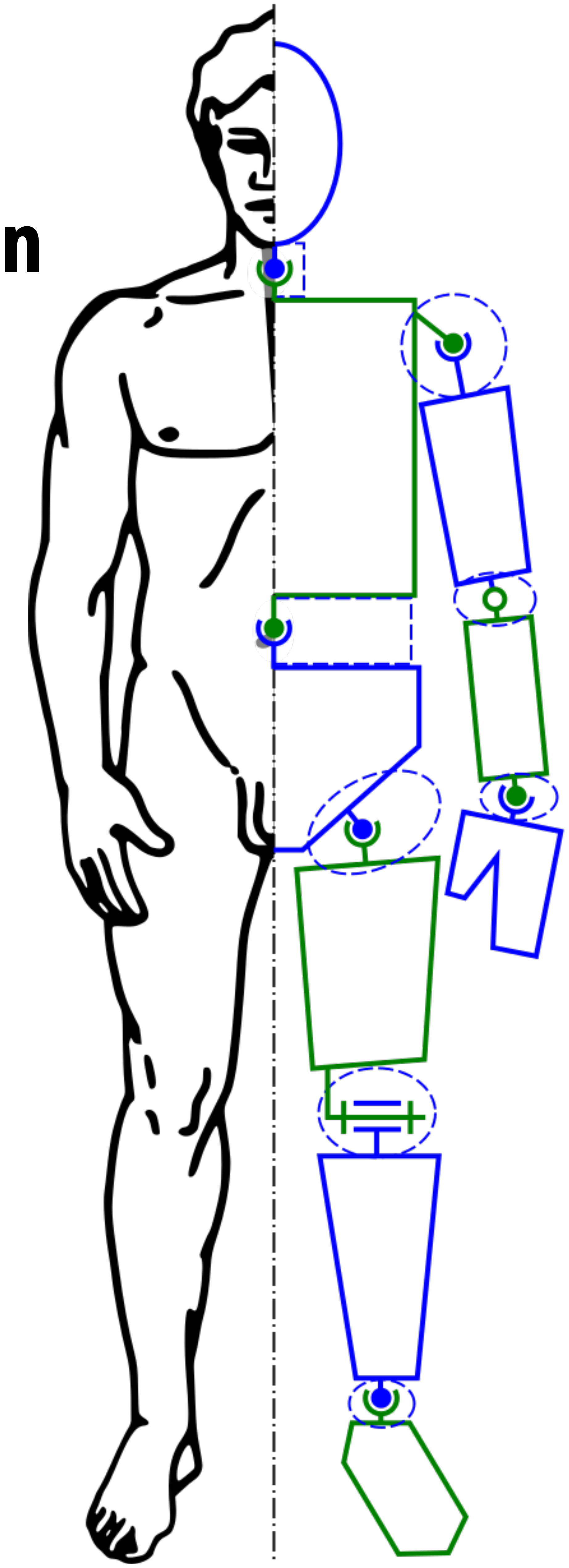
- **Great for convex problems** **(even proofs about # of steps!)**
- **For nonconvex problems, need to be more careful**
- **In general, nonconvex optimization is a BLACK ART**
- **Meta-strategy: try lots of solvers, see what works!**
  - **quasi-Newton, trust region, L-BFGS, ...**

Example: Inverse Kinematics

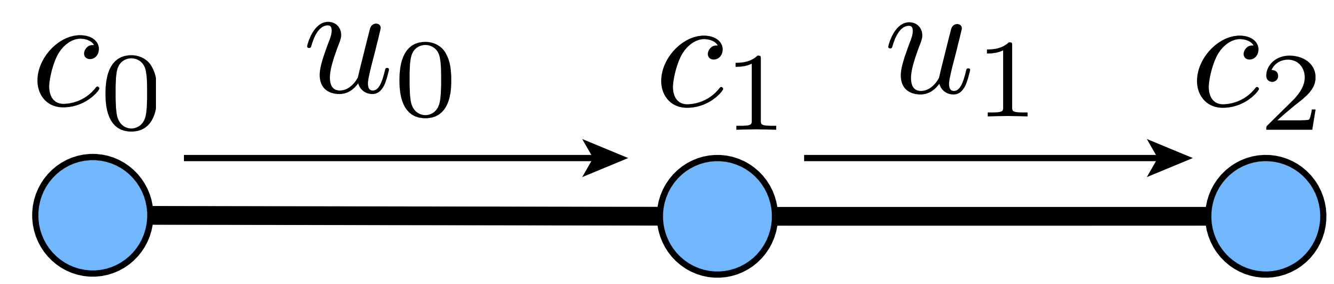


Forward Kinematics

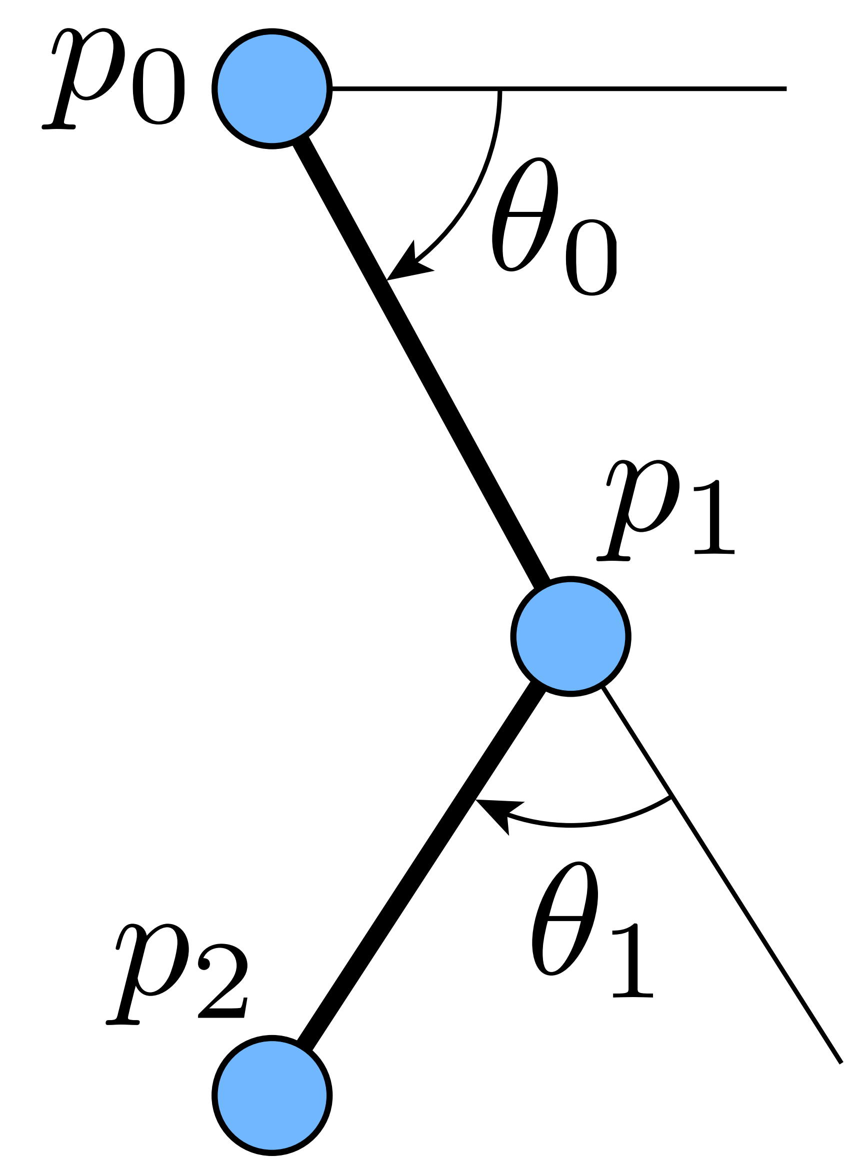
- Many systems well-described by a kinematic chain
  - collection of rigid bodies, connected by joints
  - joints have various behaviors (ball, piston, ...)
  - also have constraints (e.g., range of angles)
  - hierarchical structure (body→leg→foot)
- In animation, often called a rig
- How do we specify the configuration of a "rig"?
  - One way: artist sets each joint individually
  - Another way: ...optimization!



Simple Kinematic Chain



- **Consider a simple path-like chain in 2D**
- **Q: How do we write p_1 in terms of the root position p_0, angles, & vectors $u := c_{i+1} - c_i$?**



$$p_1 = p_0 + \begin{bmatrix} \cos\theta_0 & \sin\theta_0 \\ -\sin\theta_0 & \cos\theta_0 \end{bmatrix} u_0$$

- **(For brevity, can use complex numbers:)**

$$p_1 = p_0 + e^{\imath\theta_0} u_0$$

- **Q: How about p_2?**

$$p_2 = p_0 + e^{\imath\theta_0} u_0 + e^{\imath\theta_0} e^{\imath\theta_1} u_1$$

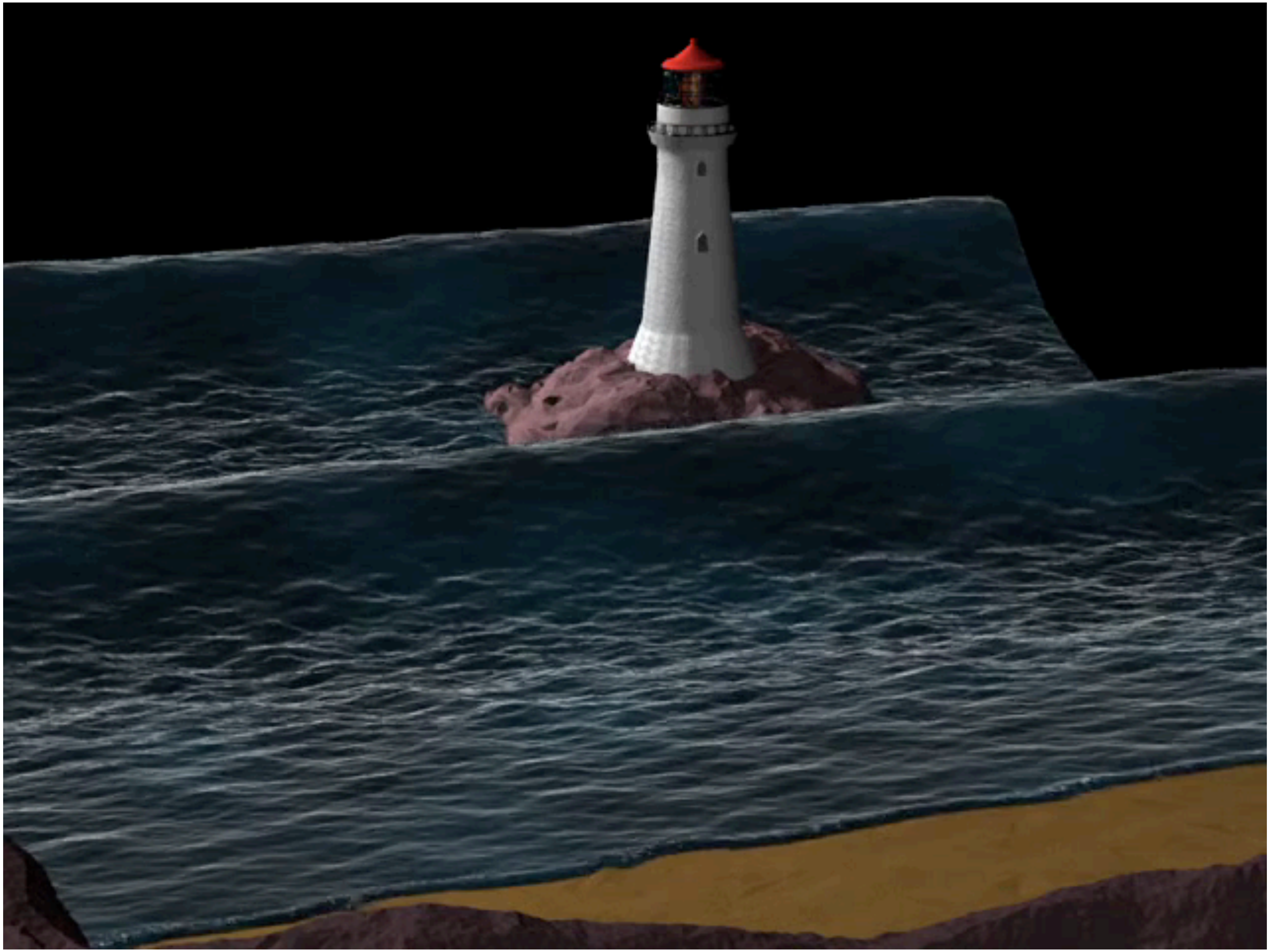
Simple IK Algorithm

- **Basic idea behind our IK algorithm:**
  - write down distance between final point and "target"
  - compute gradient with respect to angles
  - apply gradient descent
- **Objective?**

$$f_0(\theta) = \frac{1}{2}|\tilde{p}_n - p_n|^2$$

- **Constraints?**
  - None! The joint angle can take any value.
  - Though we could limit joint angles (for instance)

Coming up next: PDEs in Computer Graphics



Frank Losasso, Jerry O. Talton, Nipun Kwatra, and Ron Fedkiw, “Two-Way Coupled SPH and Particle Level Set Fluid Simulation”