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, ...

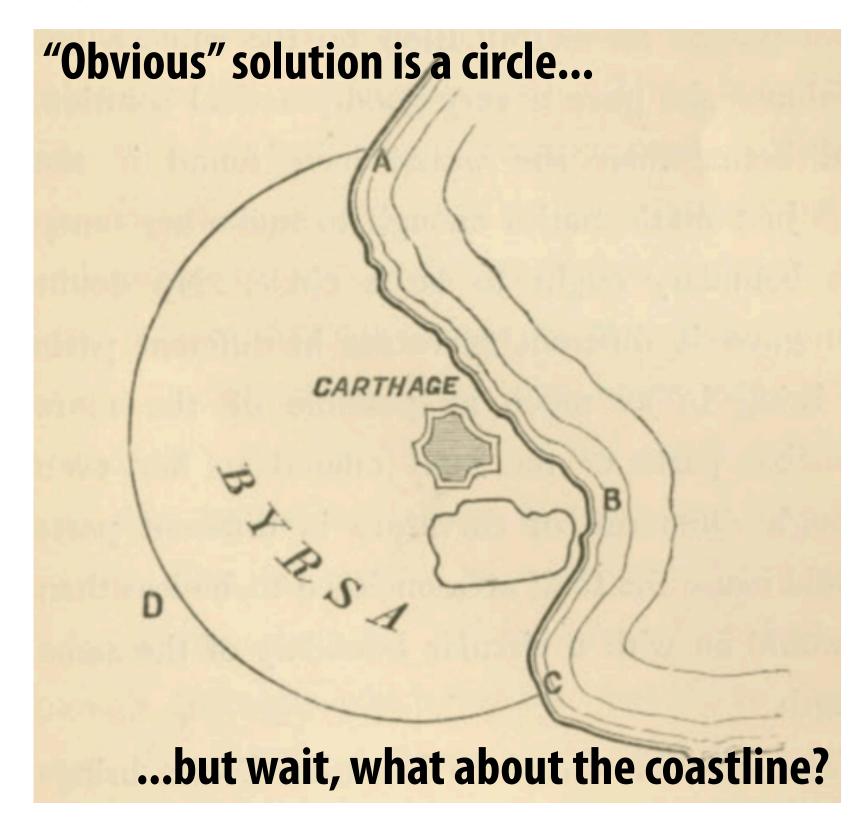


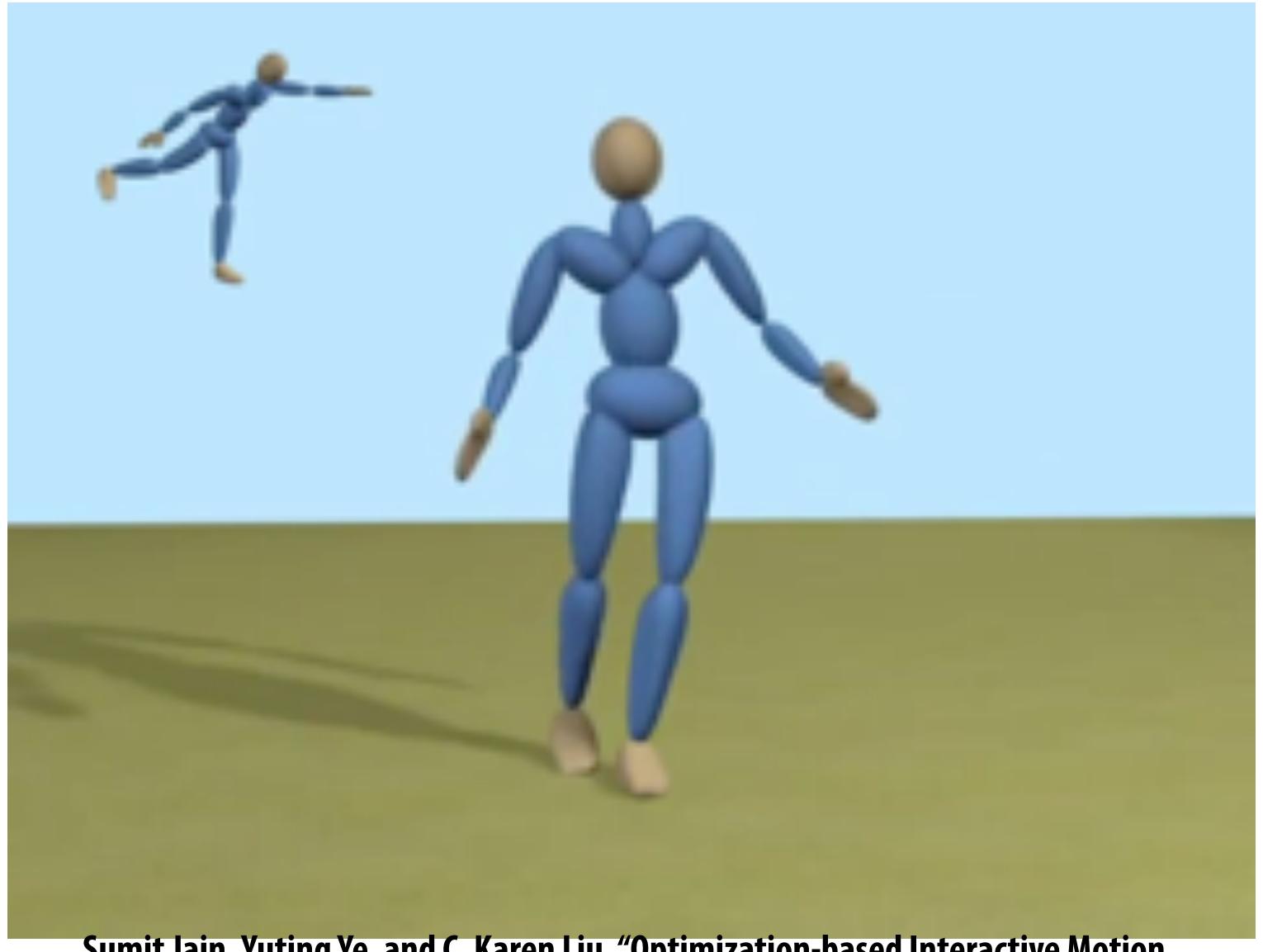
What is an optimization problem?

- 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

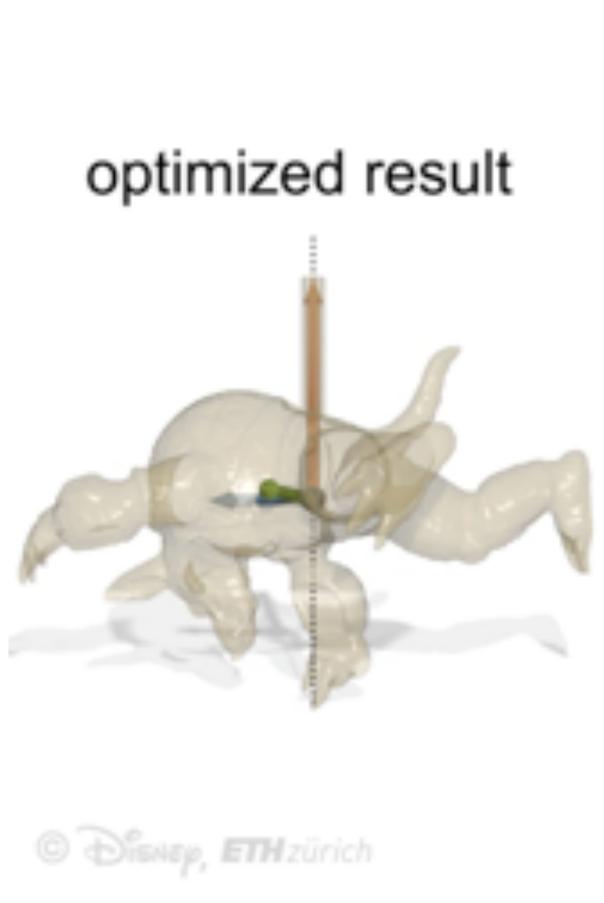


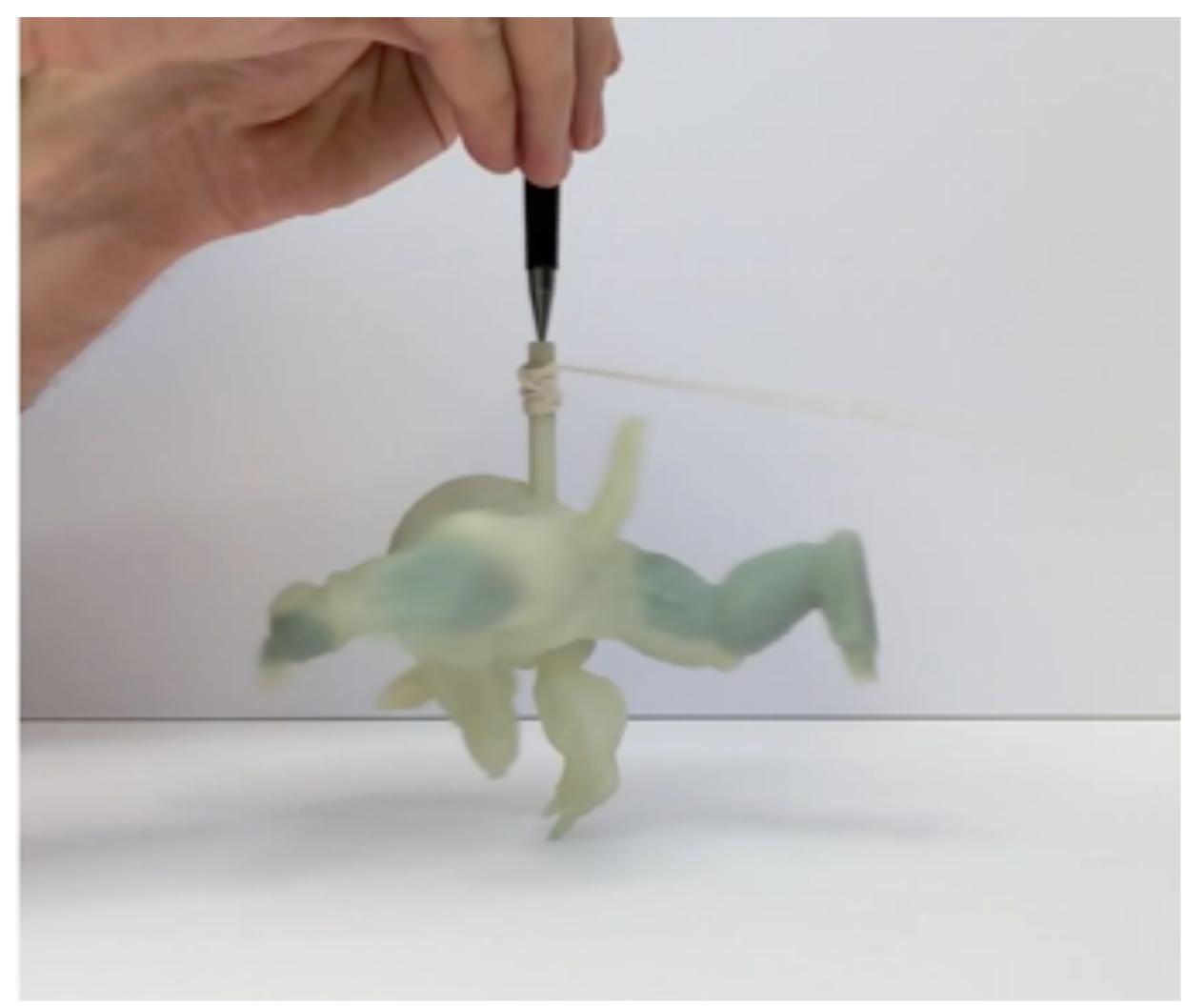


Sumit Jain, Yuting Ye, and C. Karen Liu, "Optimization-based Interactive Motion Synthesis"



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





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



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

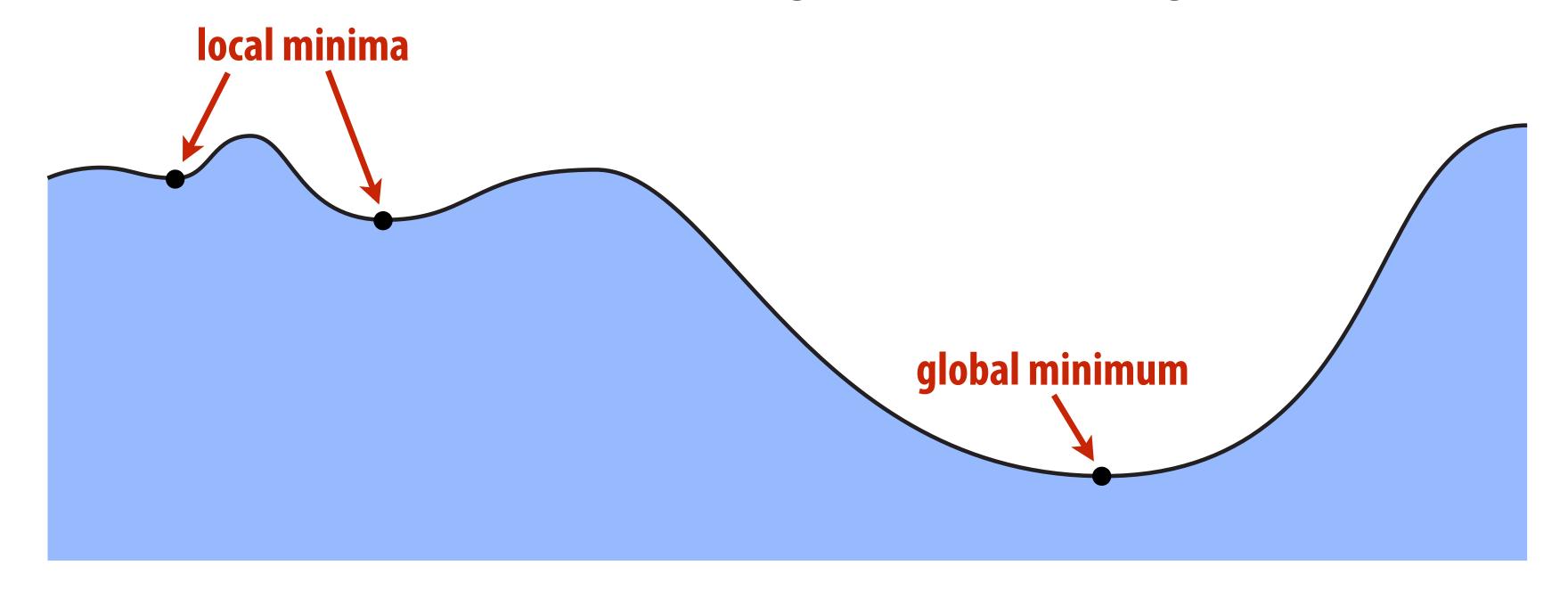
Can formulate most continuous optimization problems this way:

"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, ... $x\in\mathbb{R}^n$ subject to $f_i(x)\leq b_i,\ i=1,\dots,m$ "constraints": what must be true about x? ("x is feasible")

- Optimal solution x* has smallest value of f₀ 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: $g(x) \le c$ and $g(x) \le -c$

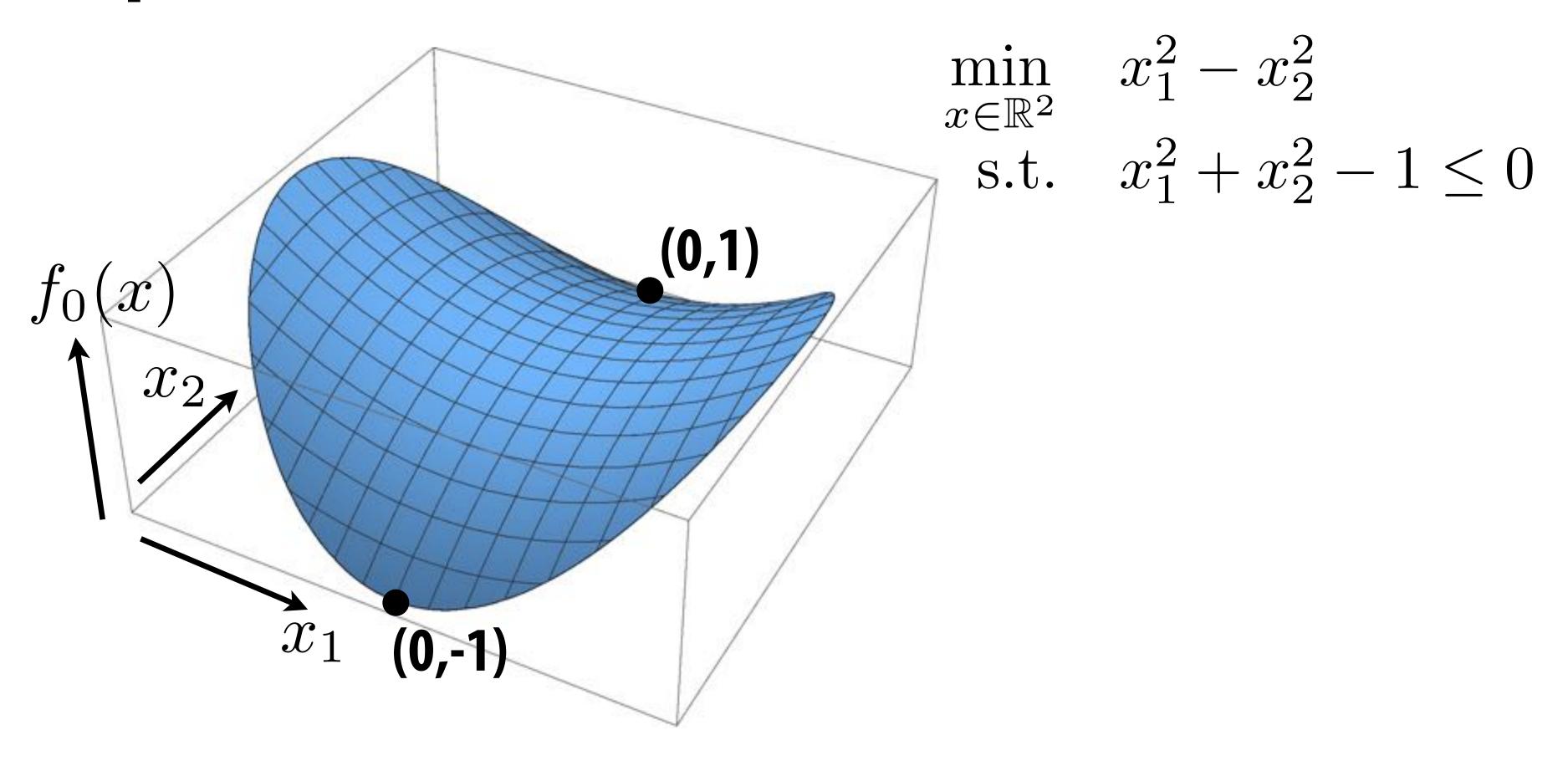
Local vs. Global Minima

- 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



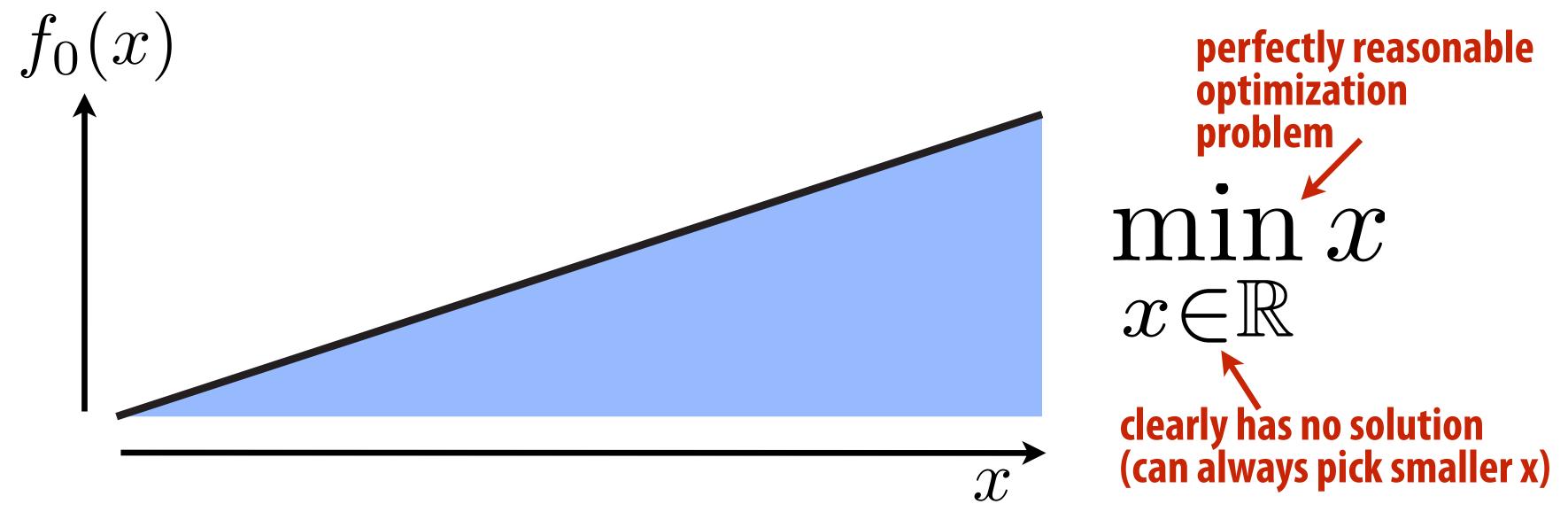
Q: Is this an optimization problem in standard form?

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?



- 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

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

- Not if there aren't any!
- problem now is just finding a feasible solution—which can be really hard (or impossible!)
- Every system of equations is an optimization problem.
- But not all problems have solutions!
- (You'll appreciate this more as you get older.)

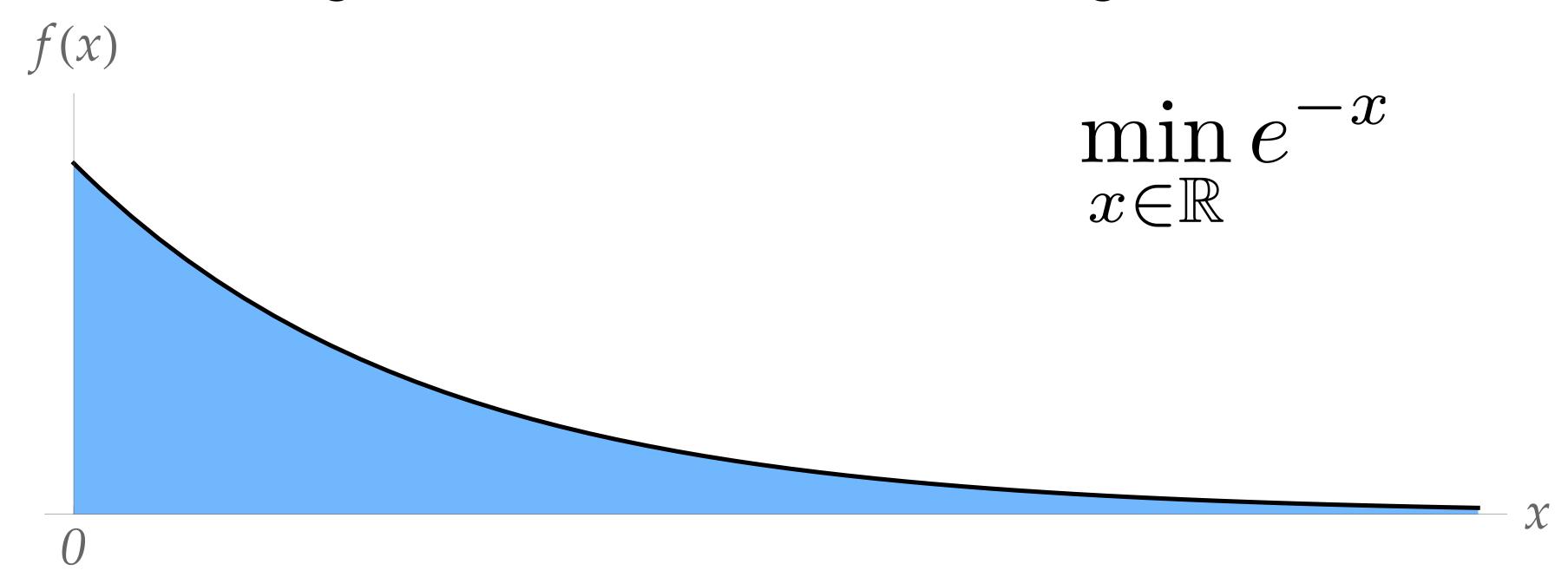
Feasibility - Example

 $\sin(x_1) + x_2^2$ Q: Is this problem feasible? min $x \in \mathbb{R}^2$ $x \in \mathbb{R}^2$ s.t. $(x_1 - 2)^2 + x_2^2 \le 1,$ $x_1 \le -1$

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

Existence & Uniqueness of Minimizers, cont.

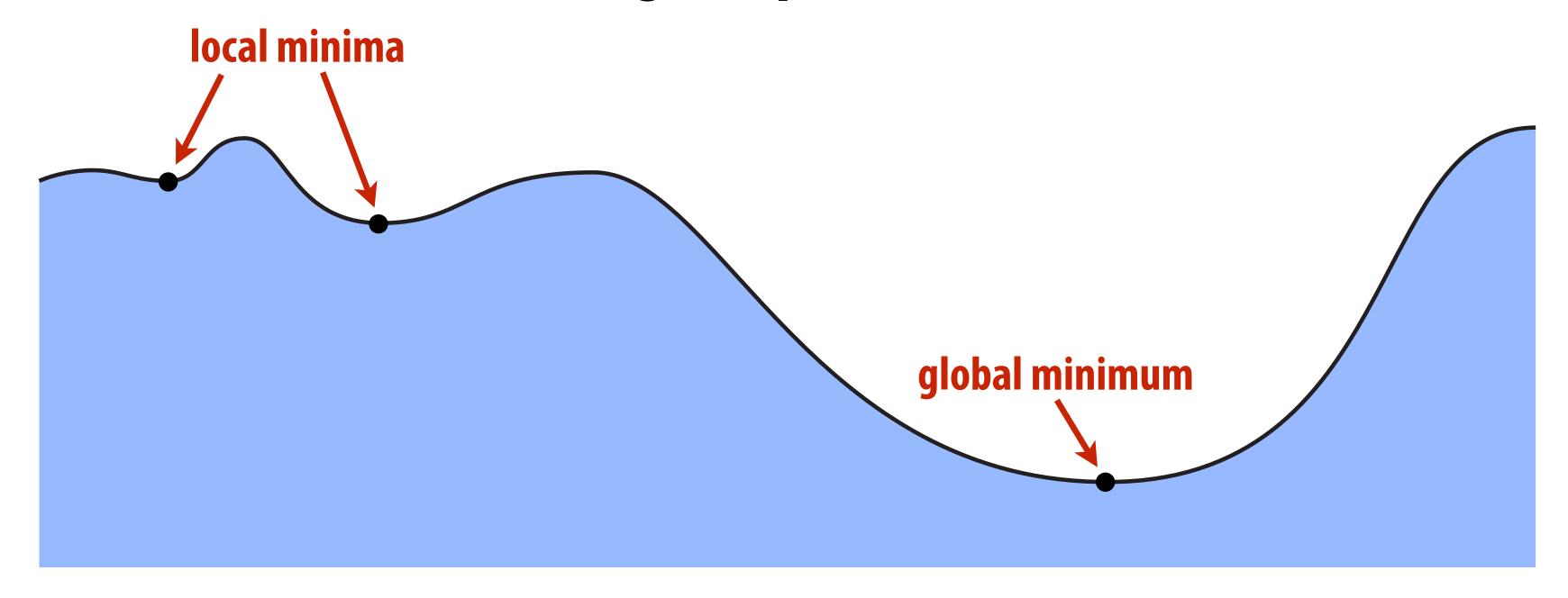
Even being bounded from below is not enough:



- 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

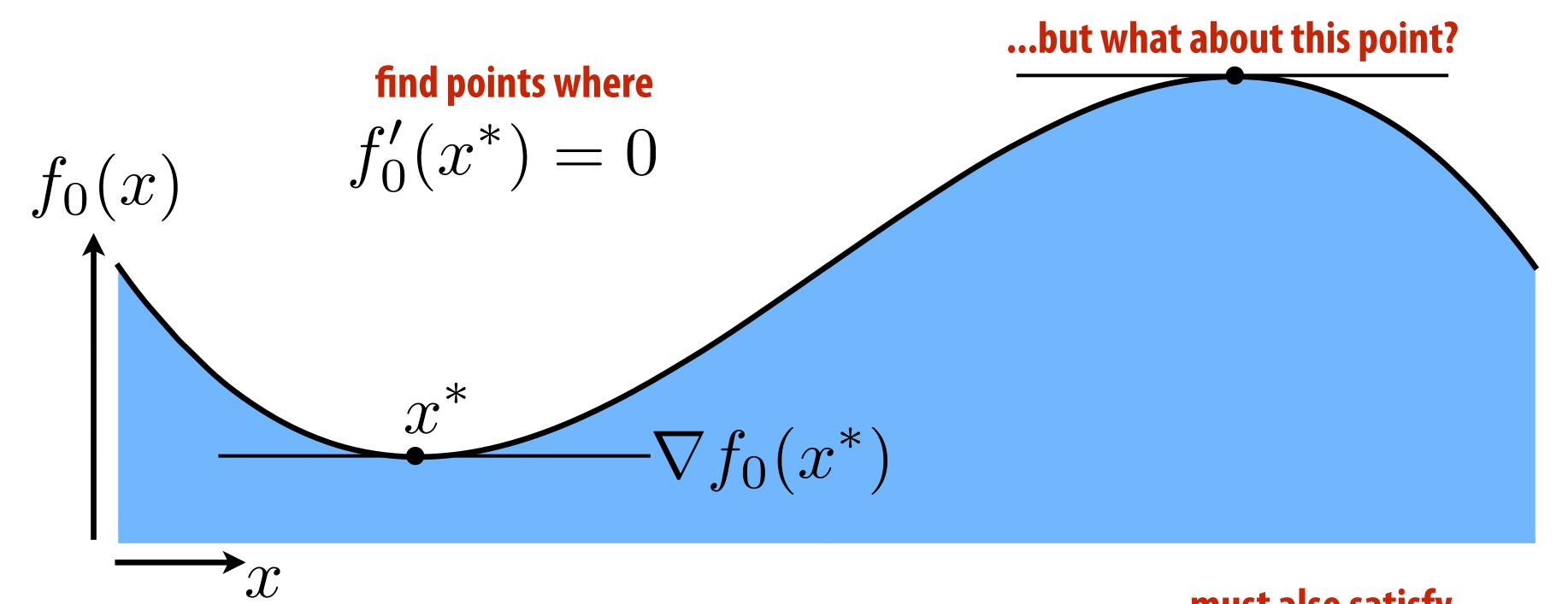
- Ok, so we have some sense of when a minimizer might exist
- But how do we know a given point x is a minimizer?



- 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 : $R \rightarrow R$. How do you find a minimum?
- (Hint: you may have memorized this formula in high school!)



Also need to check second derivative (how?)

must also satisfy
$$f_0''(x^*) \ge 0$$

- Make sure it's positive
- \blacksquare Ok, but what does this all mean for more general functions f_0 ?

Optimality Conditions (Unconstrained)

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

$$\nabla f := \begin{bmatrix} \partial f/\partial x_1 \\ \vdots \\ \partial f/\partial x_n \end{bmatrix} \qquad \nabla^2 f := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \dots & \frac{\partial f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \dots & \frac{\partial f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \dots & \frac{\partial f}{\partial x_n^2} \end{bmatrix}$$
(measures "slope")

HESSIAN (measures "curvature")

Optimality conditions?

$$\nabla f_0(x^*) = 0$$
1st order

positive semidefinite (PSD) $(\mathbf{u}^{\mathsf{T}} \mathbf{A} \mathbf{u} \ge \mathbf{0} \text{ for all } \mathbf{u})$ $\nabla^2 f_0(x^*) \succeq 0$ 2nd order

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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)

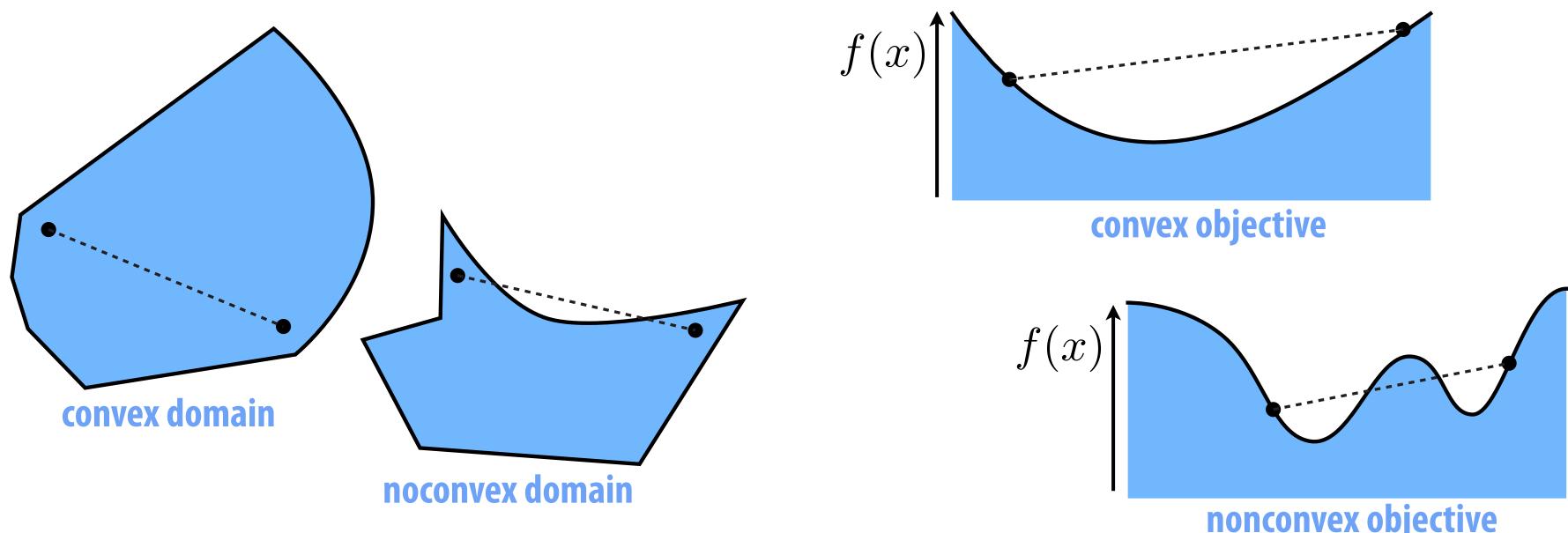


$$\exists \lambda_i \; \mathrm{s.t.} \quad
abla f_0(x^*) = -\sum_{i=1}^n \lambda_i
abla f_i(x^*) \; ext{ stationarity}$$
 $f_i(x^*) \leq 0, \; i=1,\ldots,n$ primal feasibility $\lambda_i \geq 0, i=1,\ldots,n$ dual feasibility $\lambda_i f_i(x^*) = 0, \; i=1,\ldots,n$ complementary slackness

...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



- 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!

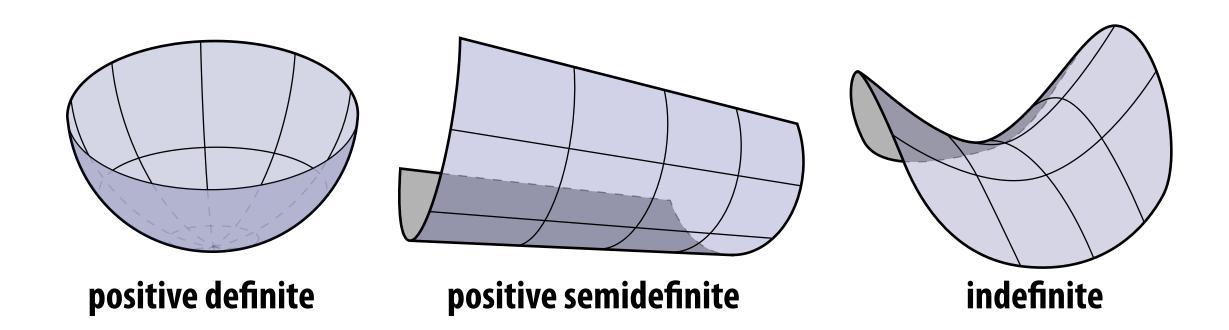
Q: 1st-order optimality condition? Ax = b

$$Ax = b$$

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?

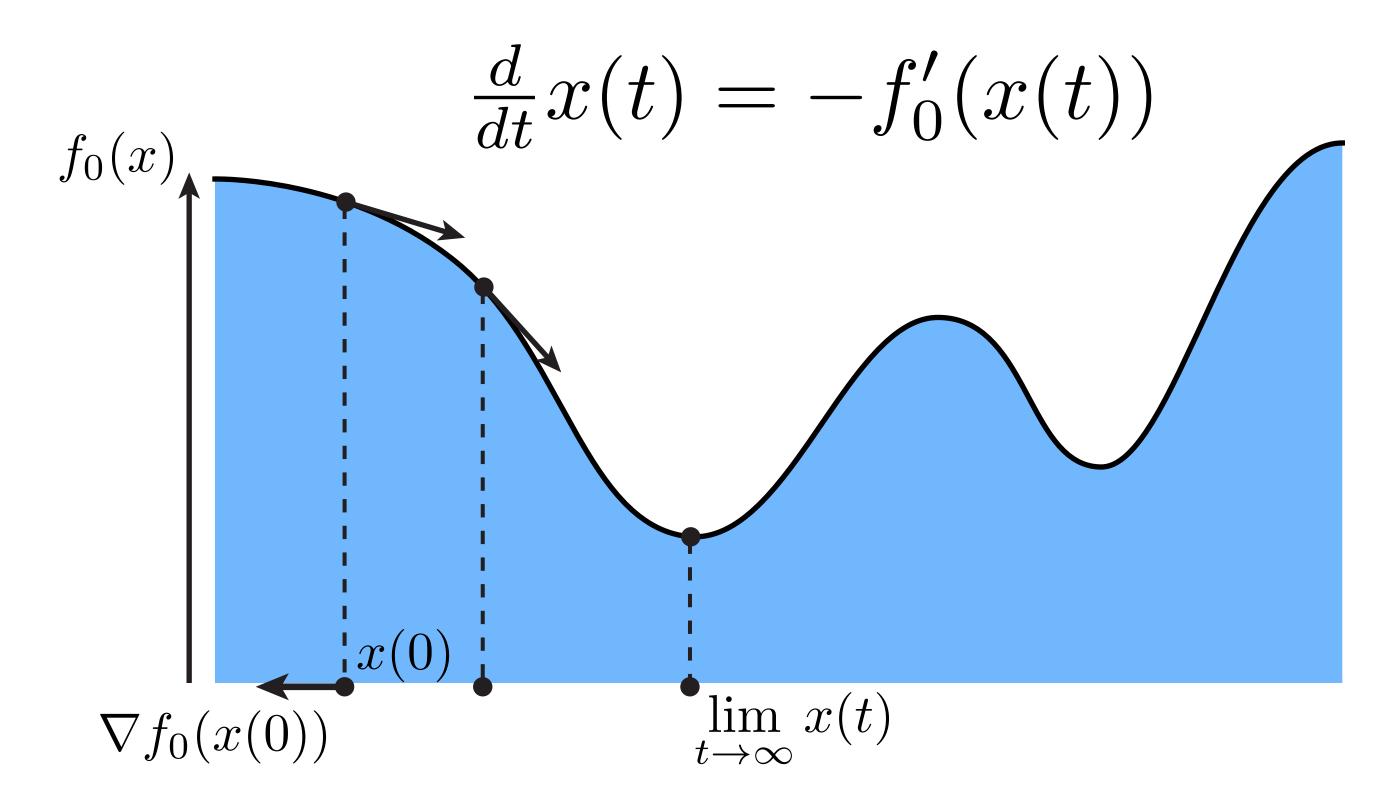
Descent Methods

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)



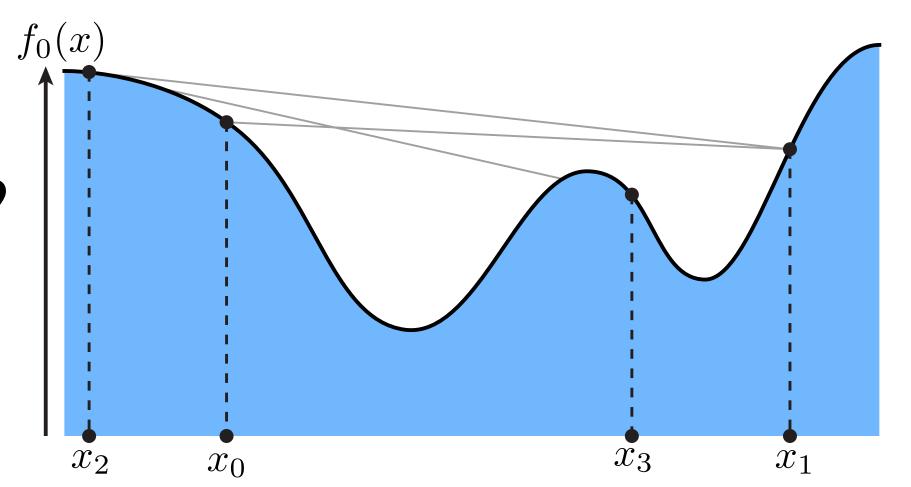
- Do we always end up at a (global) minimum?
- How do we compute gradient descent in practice?

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.
- \blacksquare For now we will do something simpler: make τ really small!

Gradient Descent Algorithm (nD)

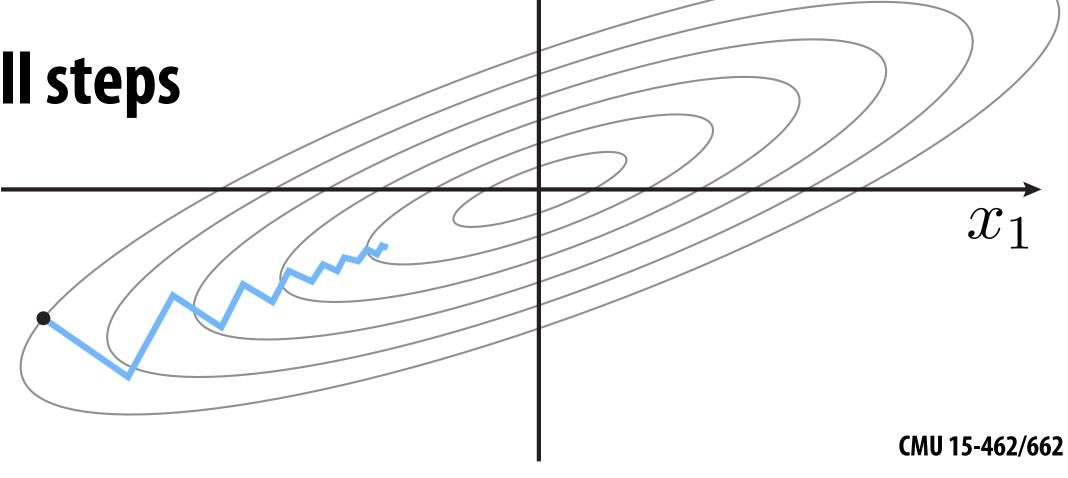
Q: How do we write gradient descent equation in general?

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

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

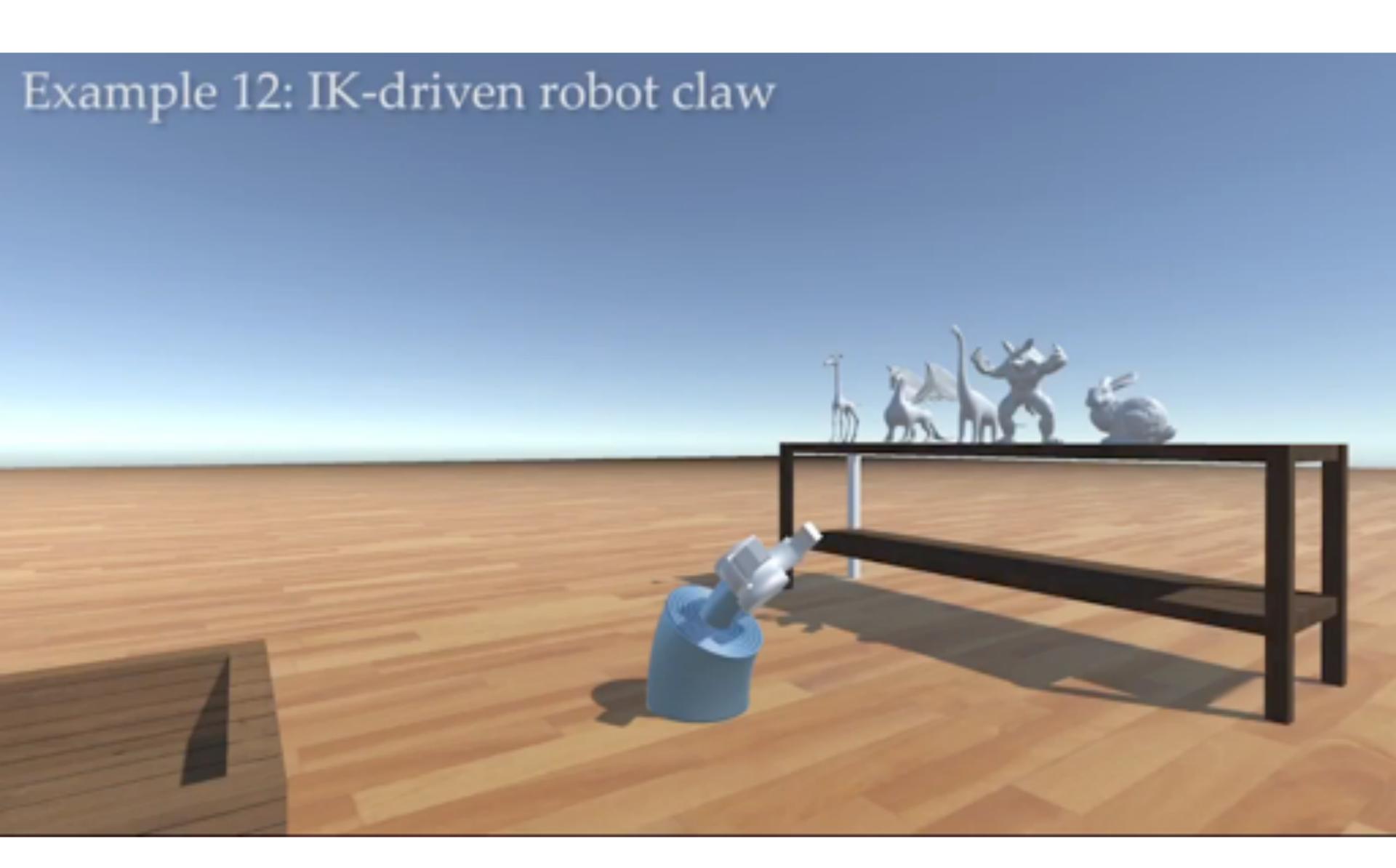
- General idea: apply a coordinate transformation so that the local energy landscape looks more like a "round bowl"
- **■** Gradient now points directly toward nearby minimizer
- Most basic strategy: Newton's method:

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



- **■** 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, ...

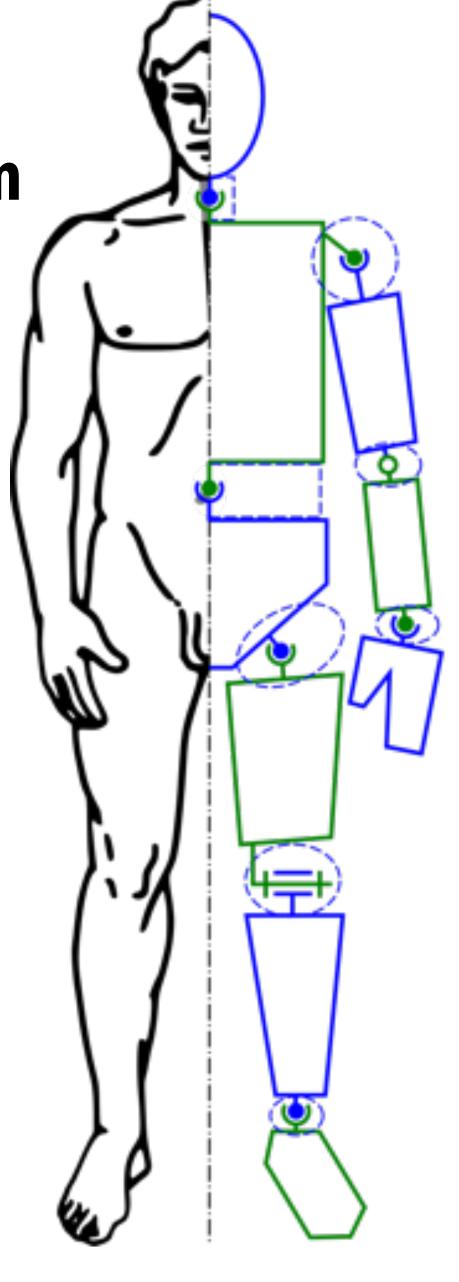
Example: Inverse Kinematics



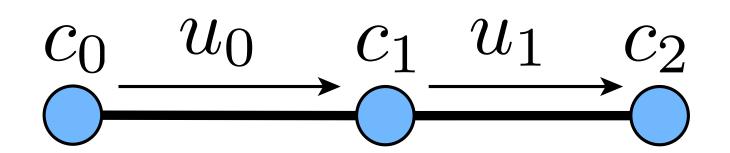
Forward Kinematics

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 $u := c_{i+1}-c_i$?

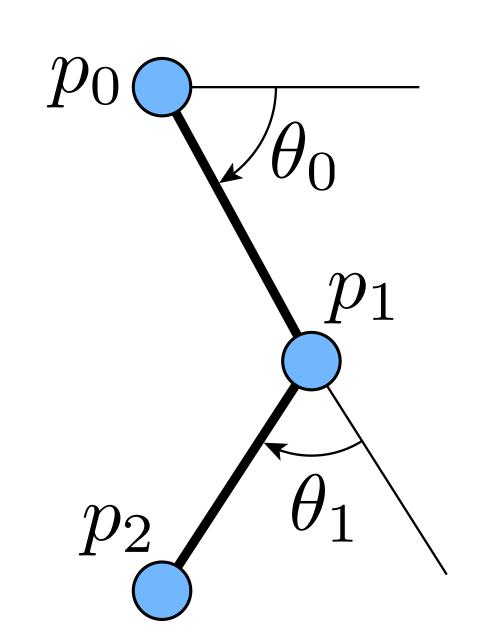
$$p_1 = p_0 + \begin{bmatrix} \cos \theta_0 & \sin \theta_0 \\ -\sin \theta_0 & \cos \theta_0 \end{bmatrix} u_0$$

(For brevity, can use complex numbers:)

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

 \blacksquare Q: How about p₂?

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



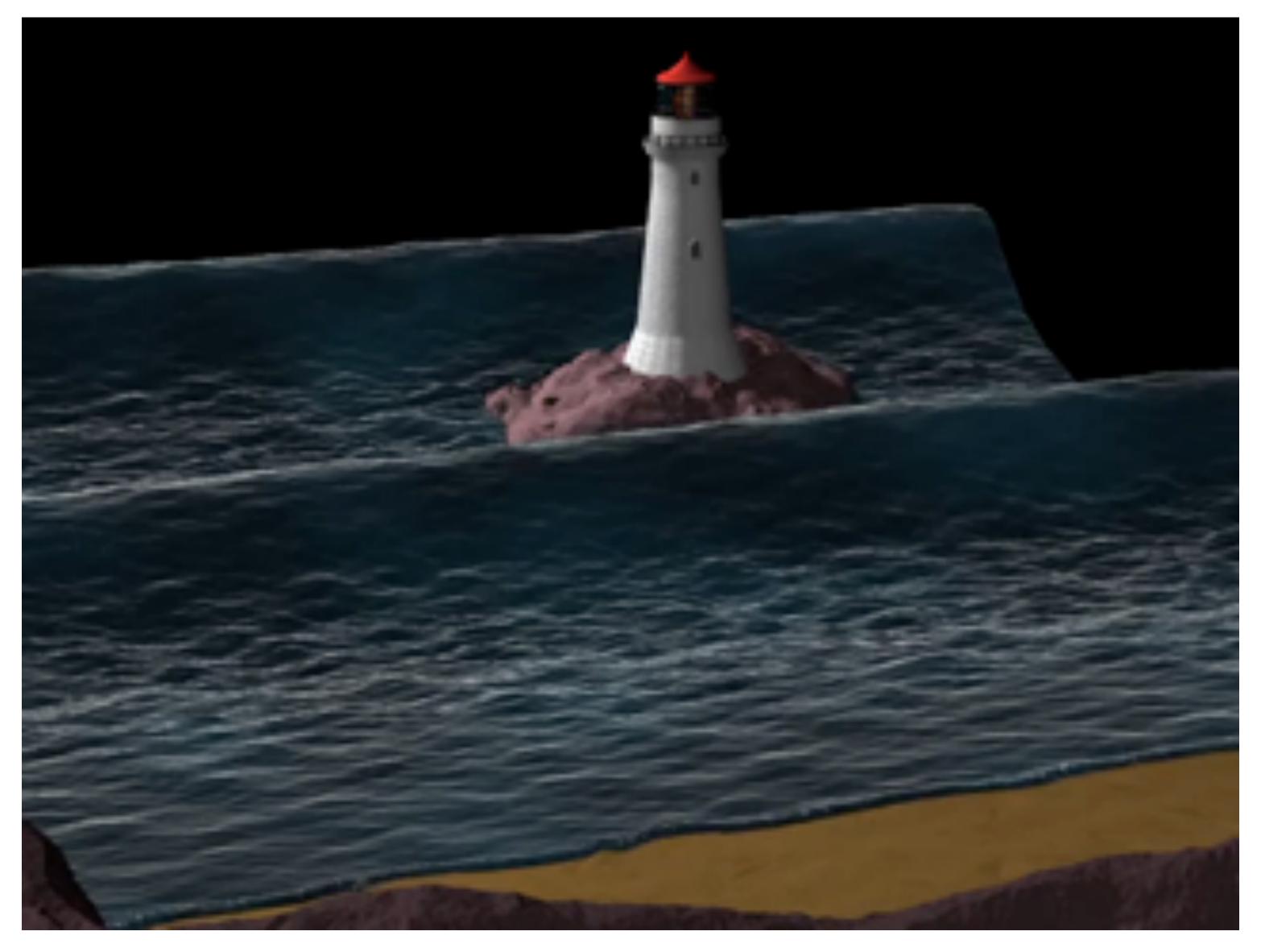
Simple IK Algorithm

- 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"