Numerical Optimization

- a brief review -

What is optimization, and why should we care about it?

Finding the best solution among all feasible options

What is an optimization problem, and why should we care about it?

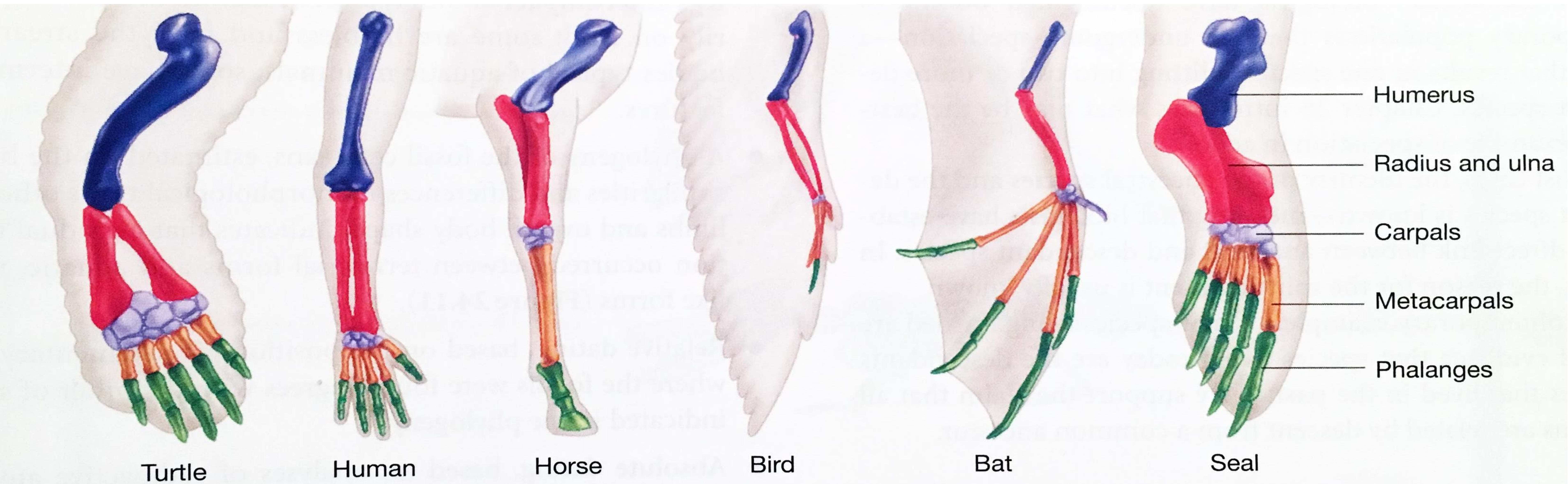
Ingredients:

- **a parameterized template/design/problem**
- **an objective/loss/reward that measures how "good" any particular point in parameter space is**
- **quite possibly some constraints**

Optimization problems are EVERYWHERE

In nature…

Find the best solution among all possibilities (subject to certain constraints)



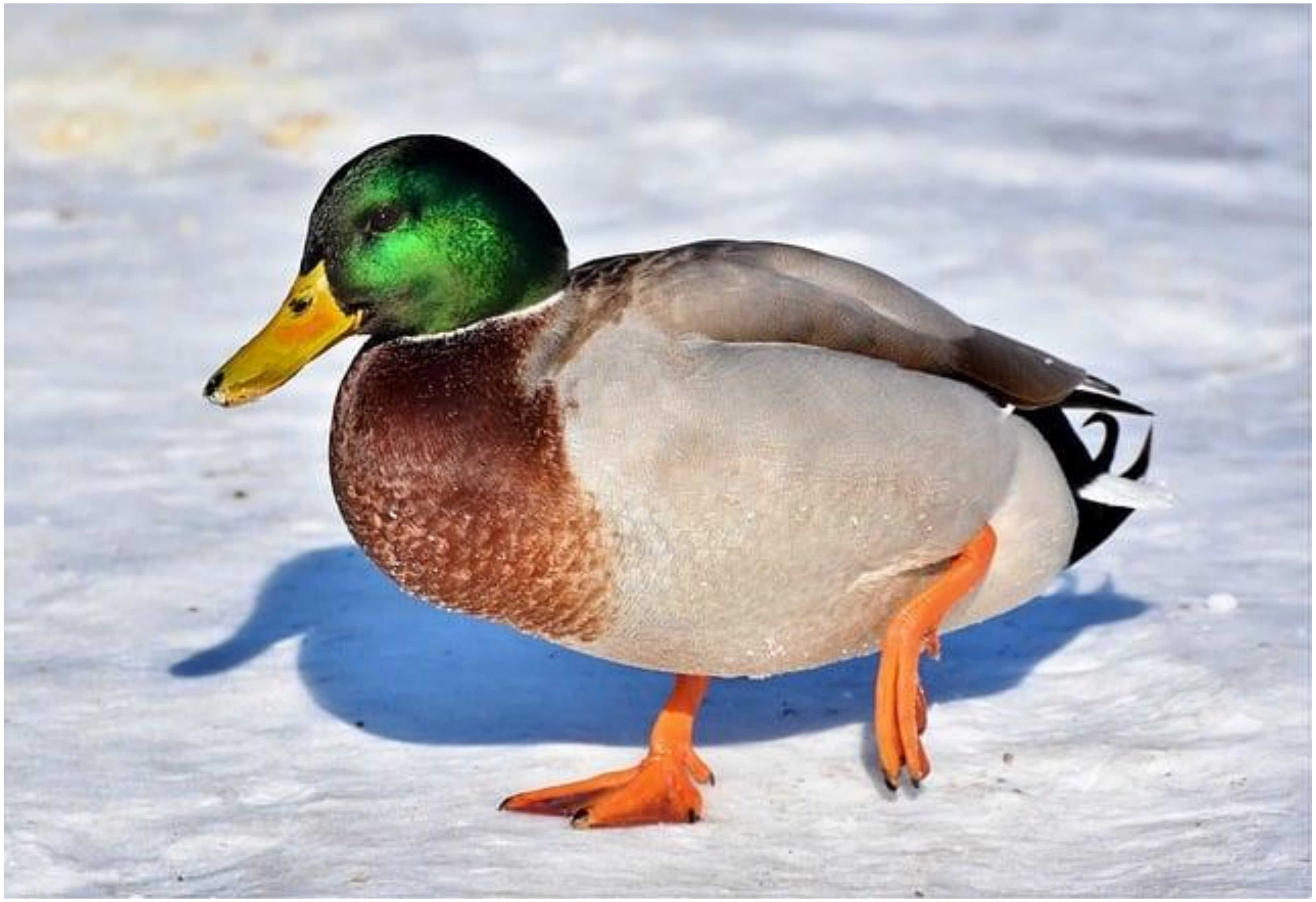
A parameterized design/template/problem

Find the best solution among all possibilities (subject to certain constraints)

Optimized for speed

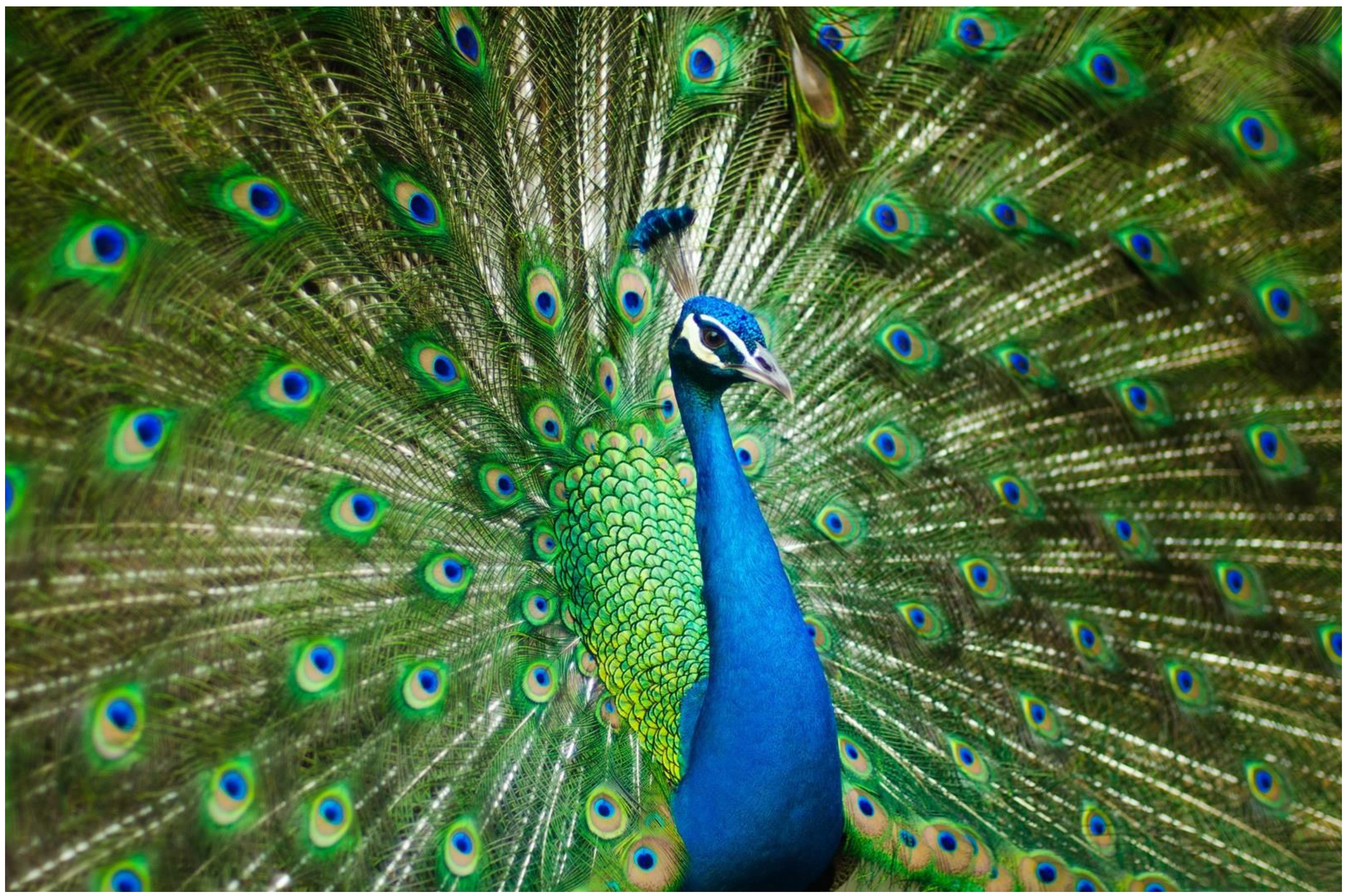
Optimized for efficiency

Find the best solution among all possibilities (subject to certain constraints)

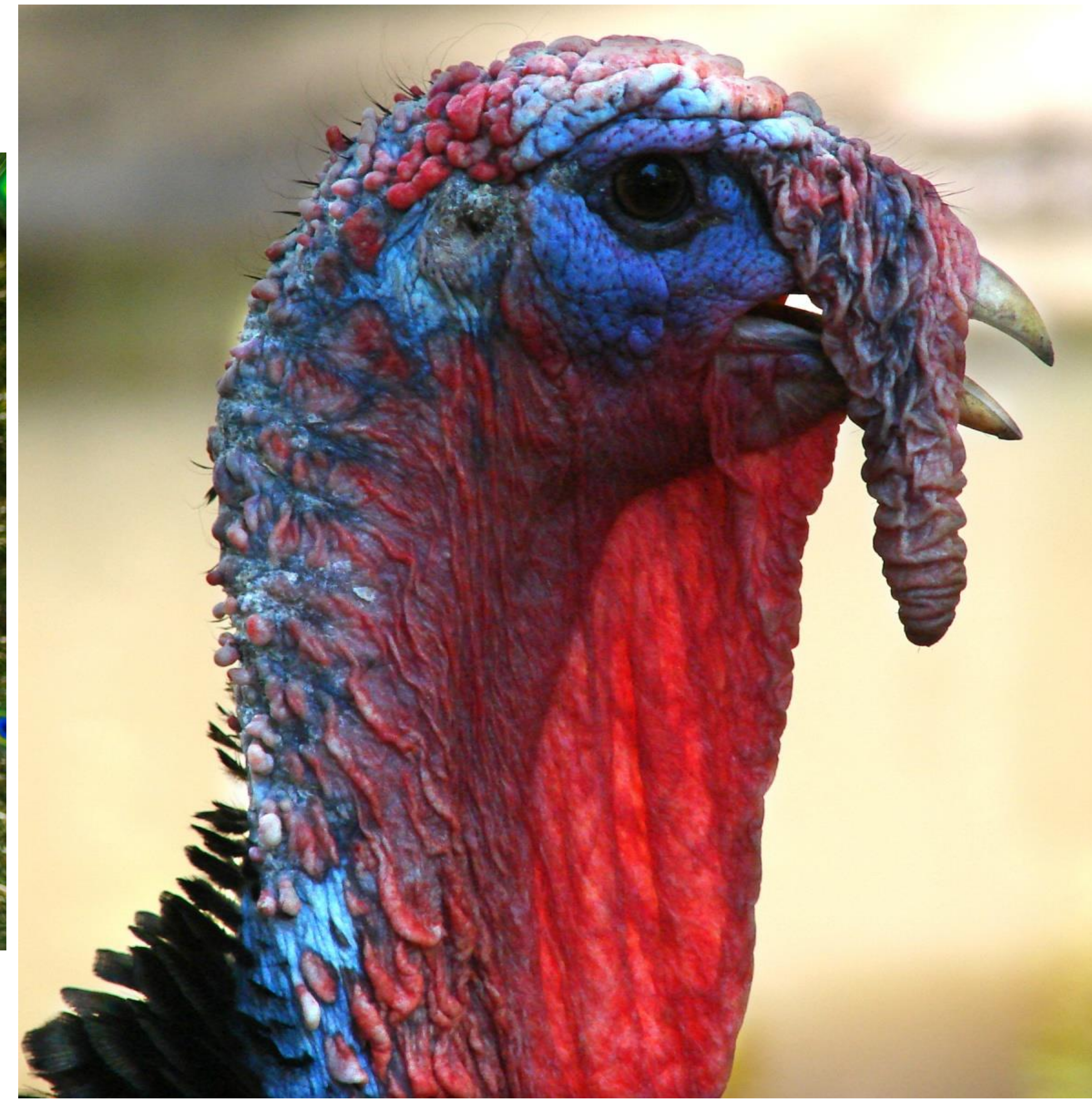


What is this optimized for?!?

Find the best solution among all possibilities (subject to certain constraints)



Optimized for beauty

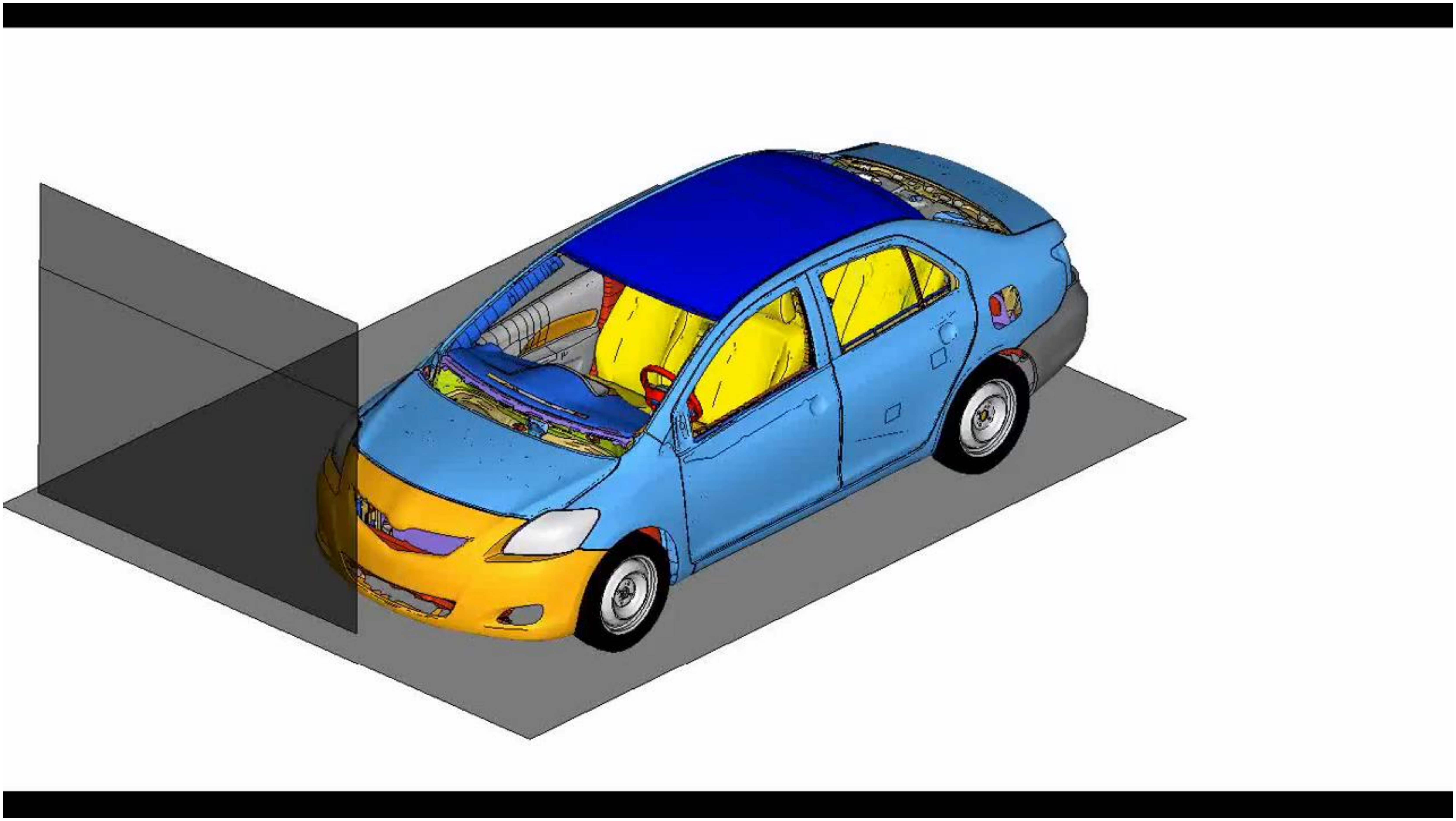


Optimized for beauty?!?

Optimization problems are EVERYWHERE

In nature…
engineering…

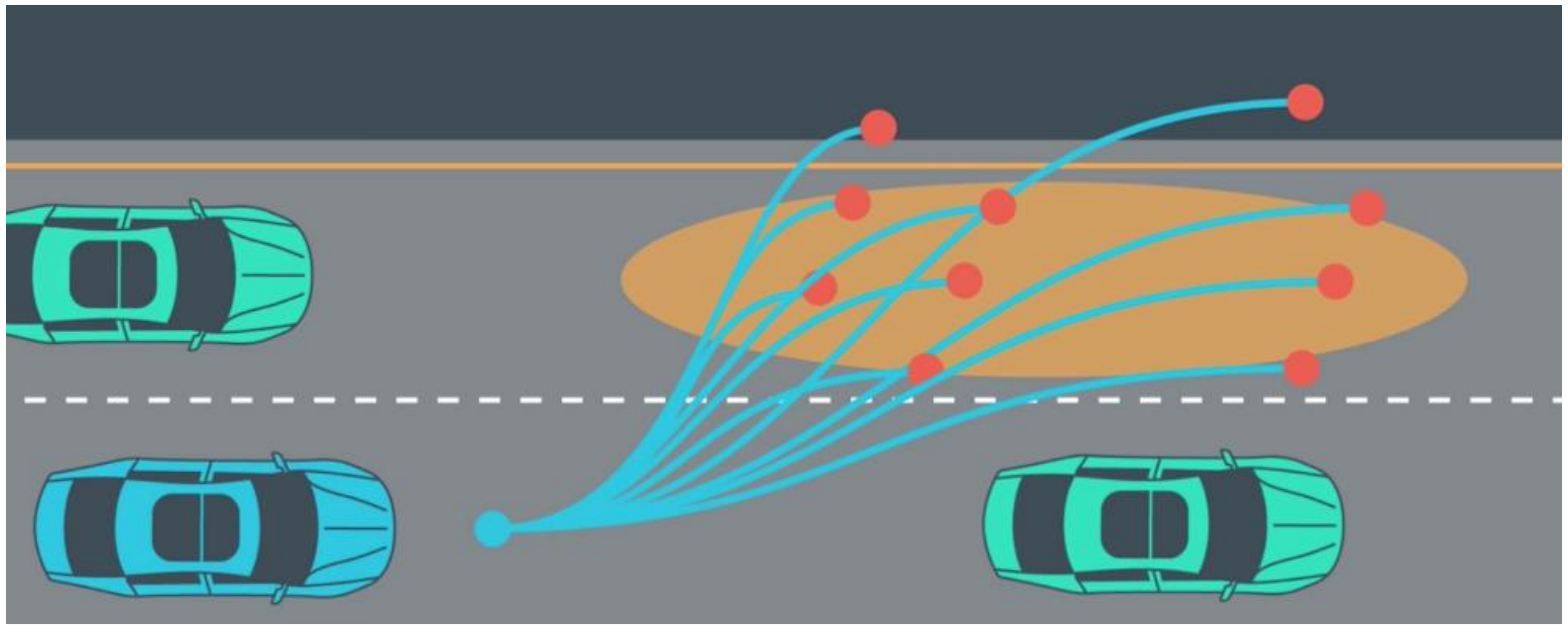
Optimization

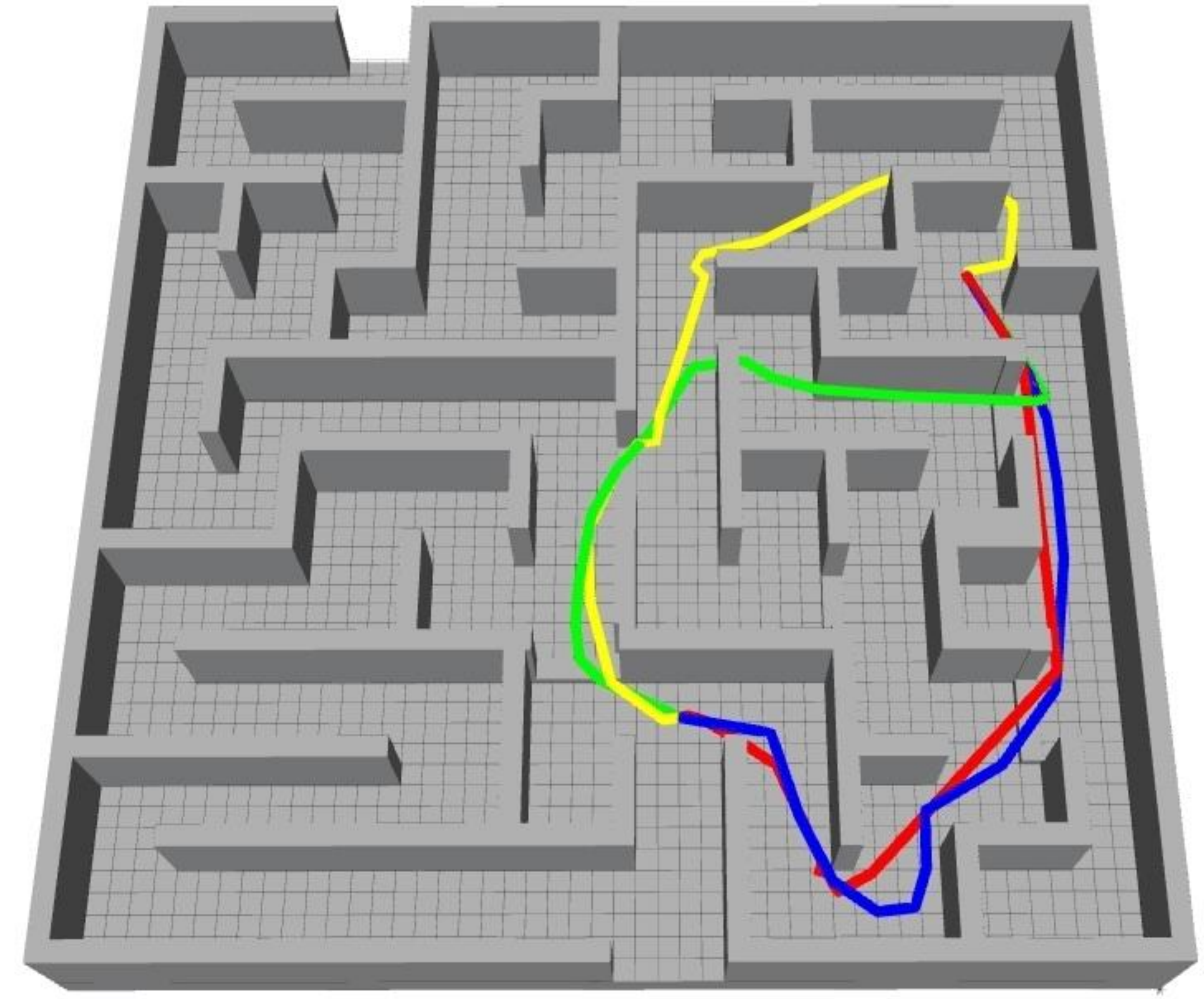


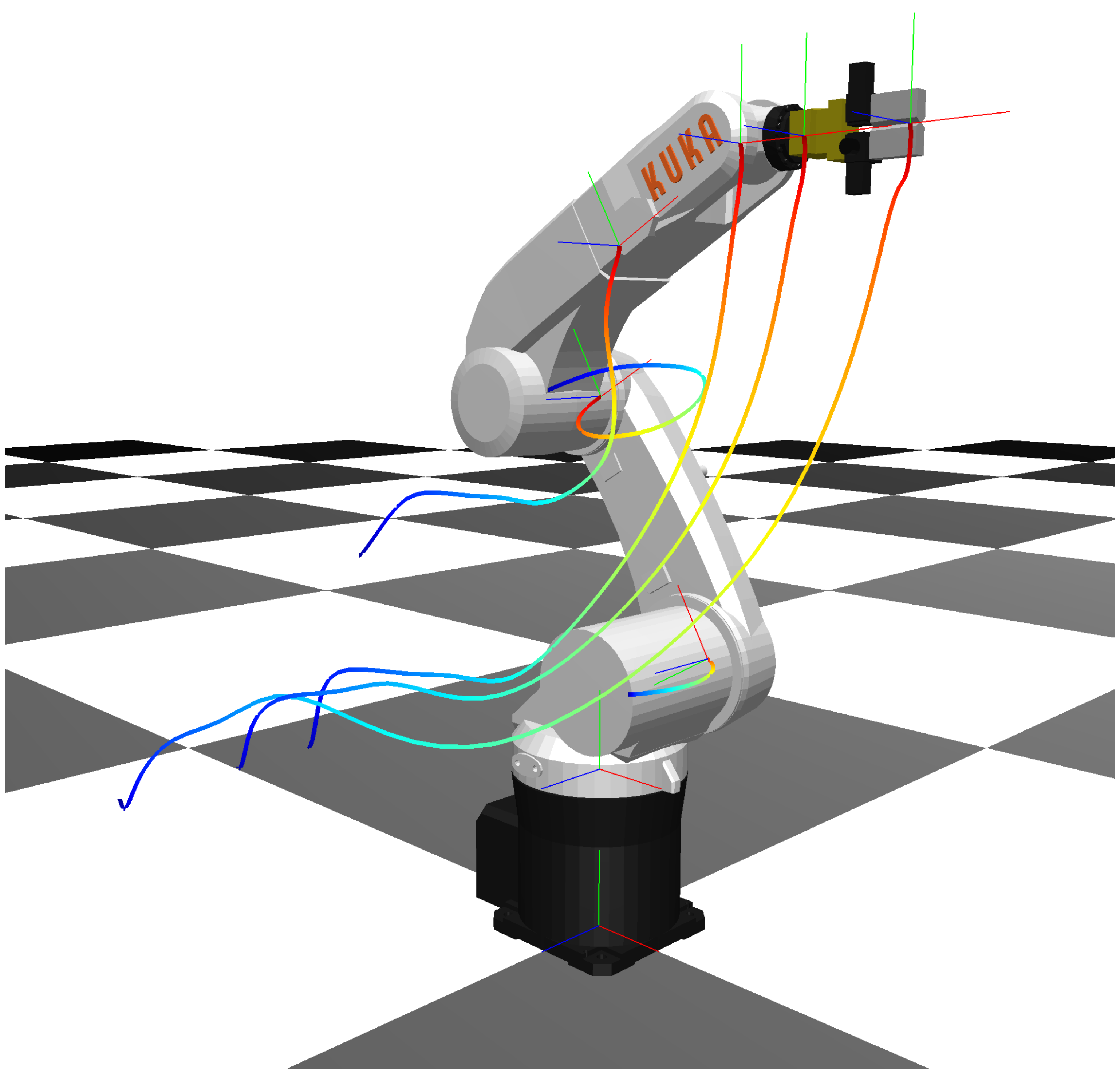
Optimization problems are EVERYWHERE

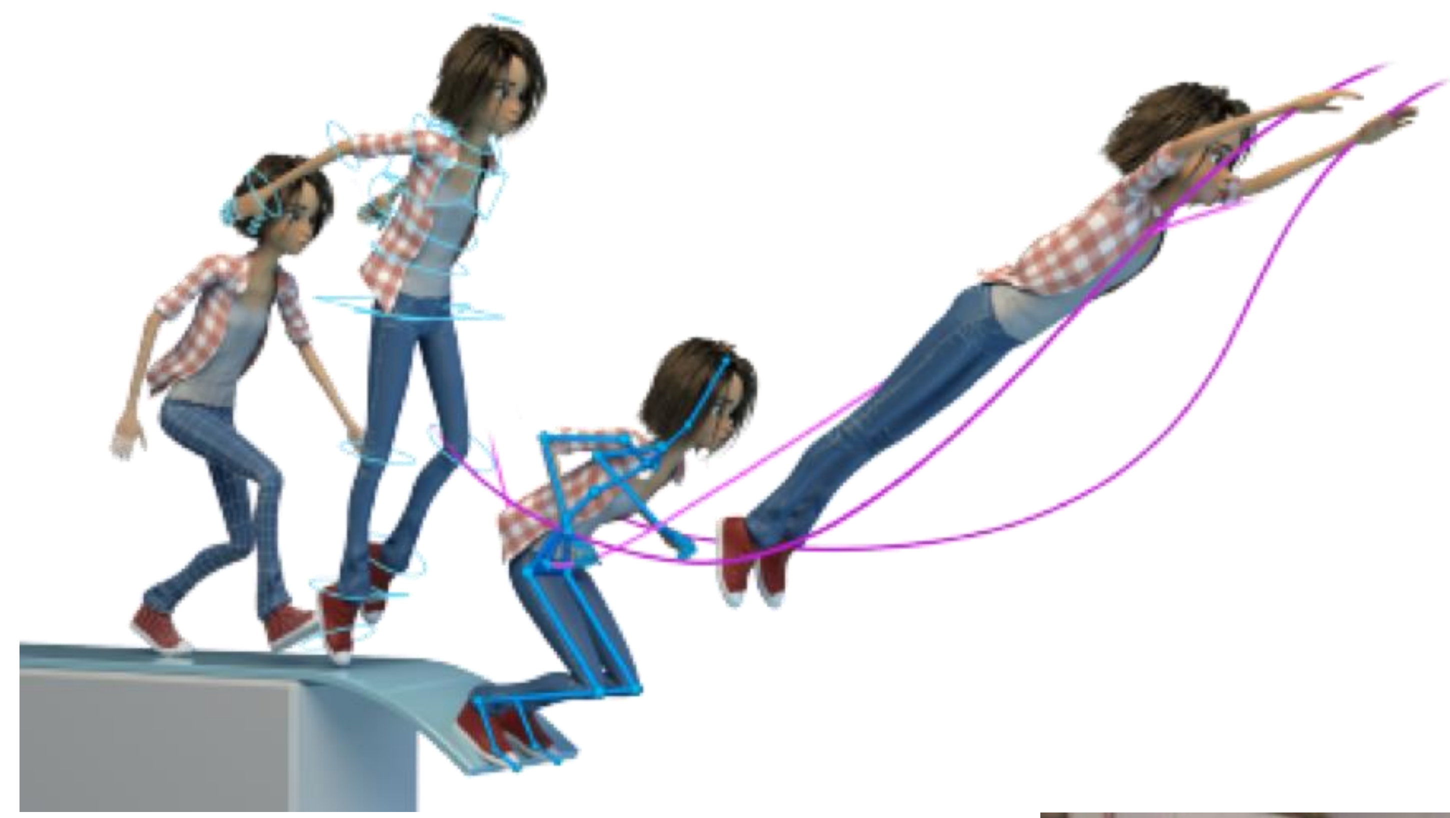
In nature…
engineering…
animation and robotics…

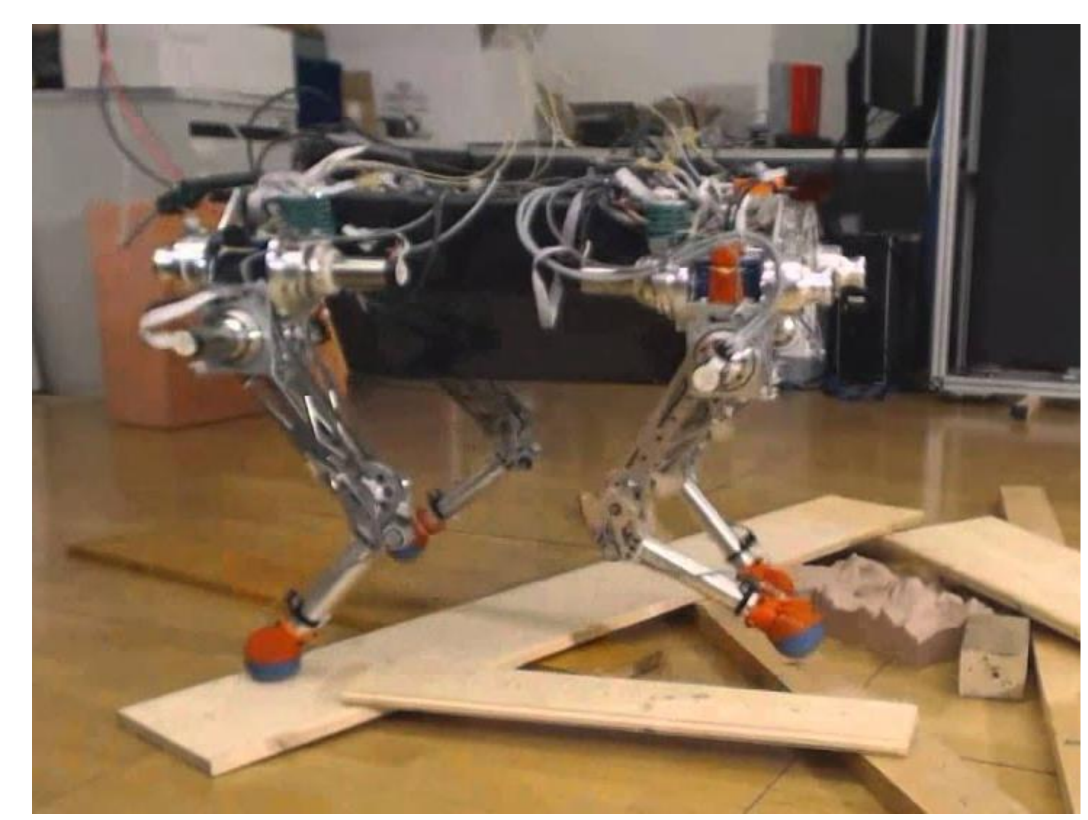
Optimization











Optimization problems are EVERYWHERE

In nature…
engineering…
animation and robotics…
machine learning…
architecture…
manufacturing…
economics…
psephology…

Knowing how to solve optimization problems is very, very useful!

Continuous vs. Discrete Optimization

- DISCRETE:
  - domain is a discrete set (e.g. integers)
  - Example: knapsack problem, lego structures, etc.
    - Basic strategy? Try all combinations! (exponential)
    - sometimes clever strategy or useful heuristics
    - can sometimes turn discrete variables into continuous ones
    - more often, NP-hard (e.g., TSP)
- CONTINUOUS:
  - domain is not discrete (e.g., real numbers)
  - still many (NP-)hard problems, but also large classes of “easy” problems (e.g., convex)
  - Gradient information, if available, is very useful

Optimization Problem in Standard Form

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

"objective": how much does solution x cost?

$$\min_{x \in \mathbb{R}^n} \quad f_0(x)$$

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

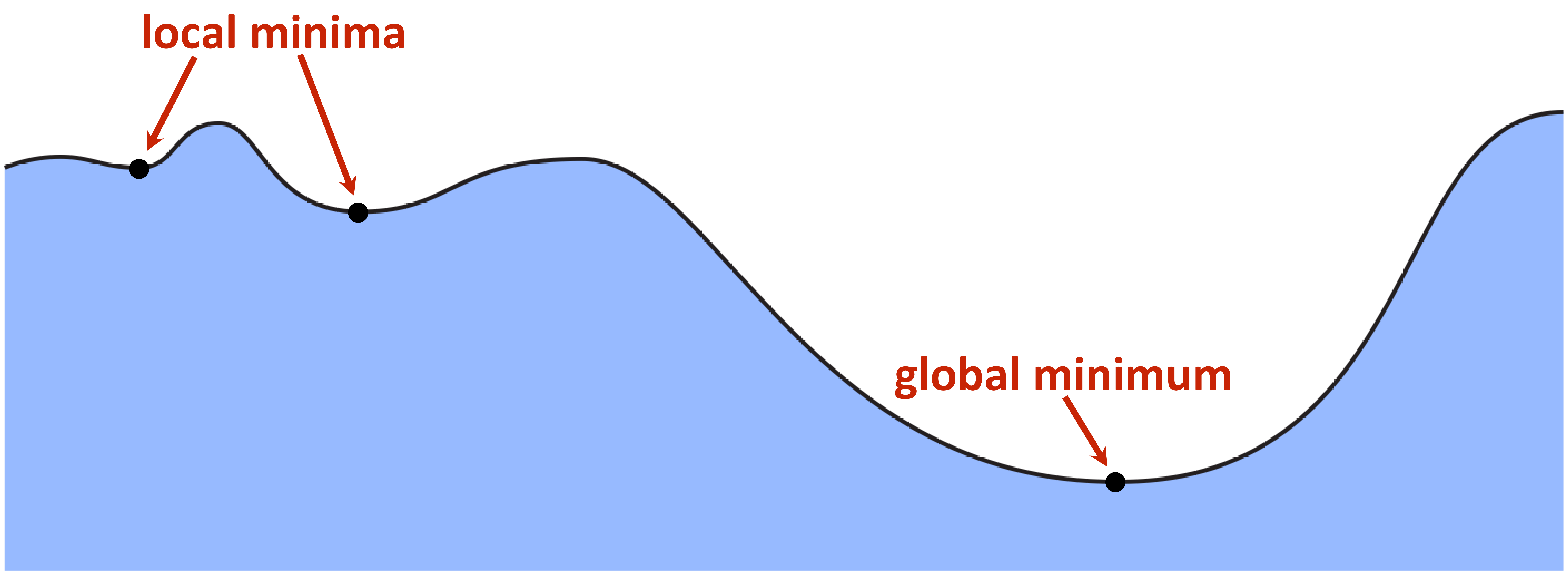
often (but not always) continuous, differentiable, ...

"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!**

Local vs. Global Minima

- *Global* minimum is absolute best among all possibilities
- *Local* minimum is best "among immediate neighbors"



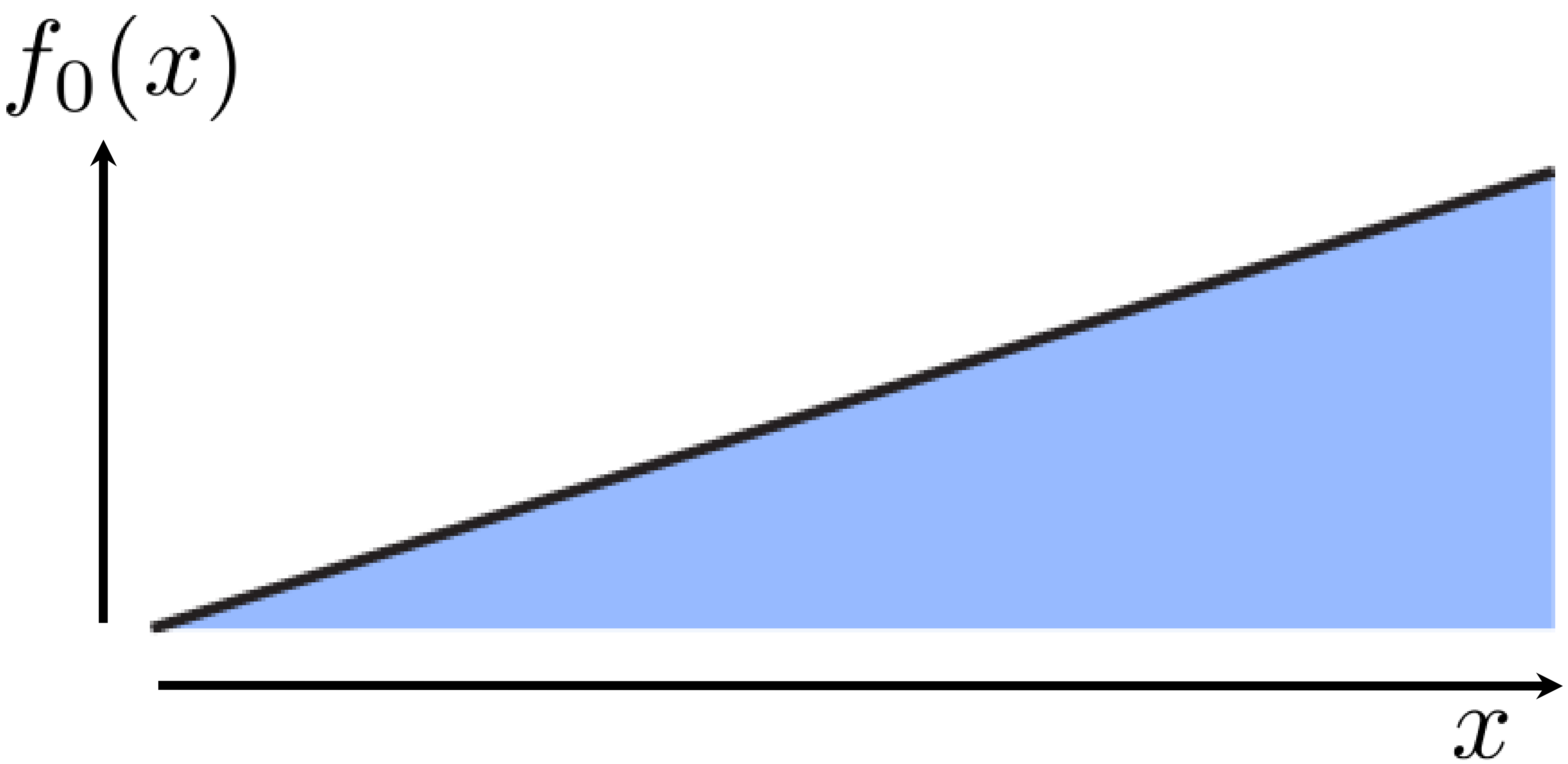
Philosophical question: does a local minimum *"solve"* the problem?

Depends on the problem! (E.g., evolution)

But sometimes, local minima can be really bad…

Existence & Uniqueness of Minimizers

- Minimizers (global or local) need not be unique.
- But is there always one? Why?
- Just consider all possibilities and take the smallest one, right?



perfectly reasonable optimization *problem*

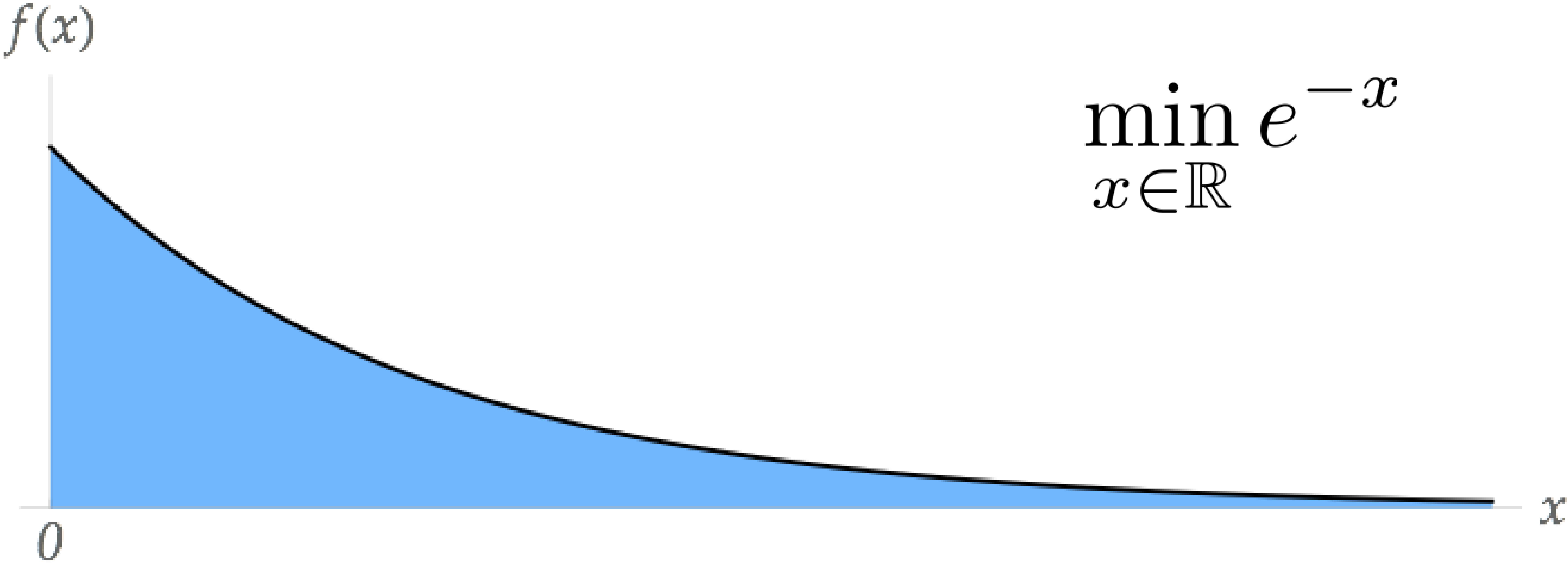
$$\min_{x \in \mathbb{R}} x$$

clearly has no *solution* (can always pick smaller x)

- Not all objectives are bounded from below.

Existence & Uniqueness of Minimizers, cont.

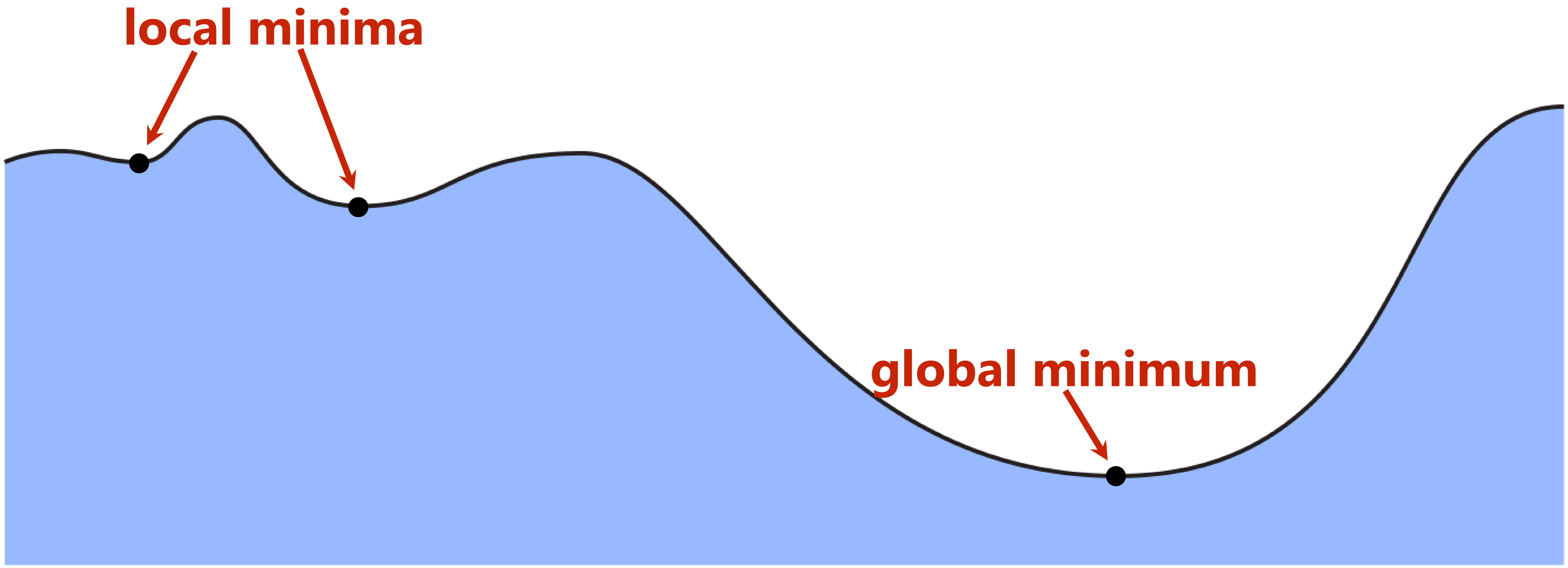
- **Even being bounded from below is not enough:**



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

Characterization of Minimizers

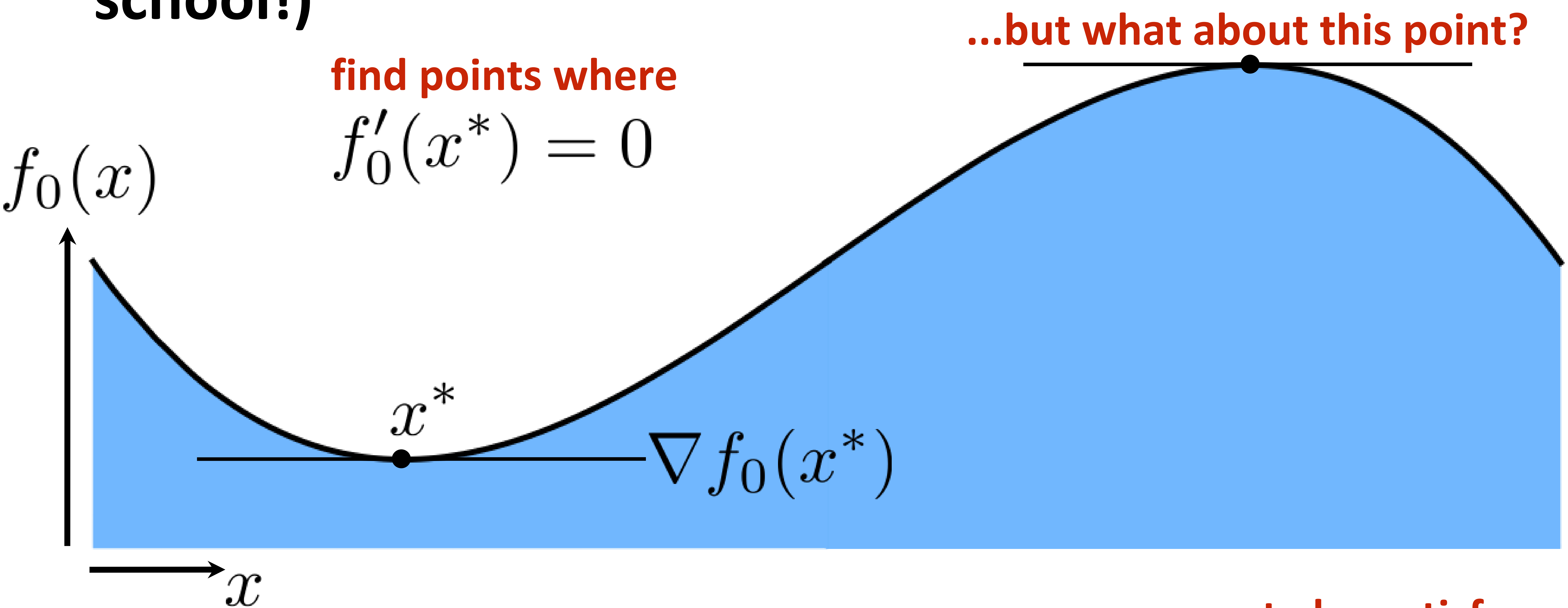
- Ok, so we have some sense of when a minimizer might *exist*
- But how do we know a given point x is a minimizer?



- 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 probably 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 (higher dimensions)

- **In general, our objective is f0: $R^n \rightarrow R$**
- **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?**

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

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

1st order

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

2nd order

Hessian

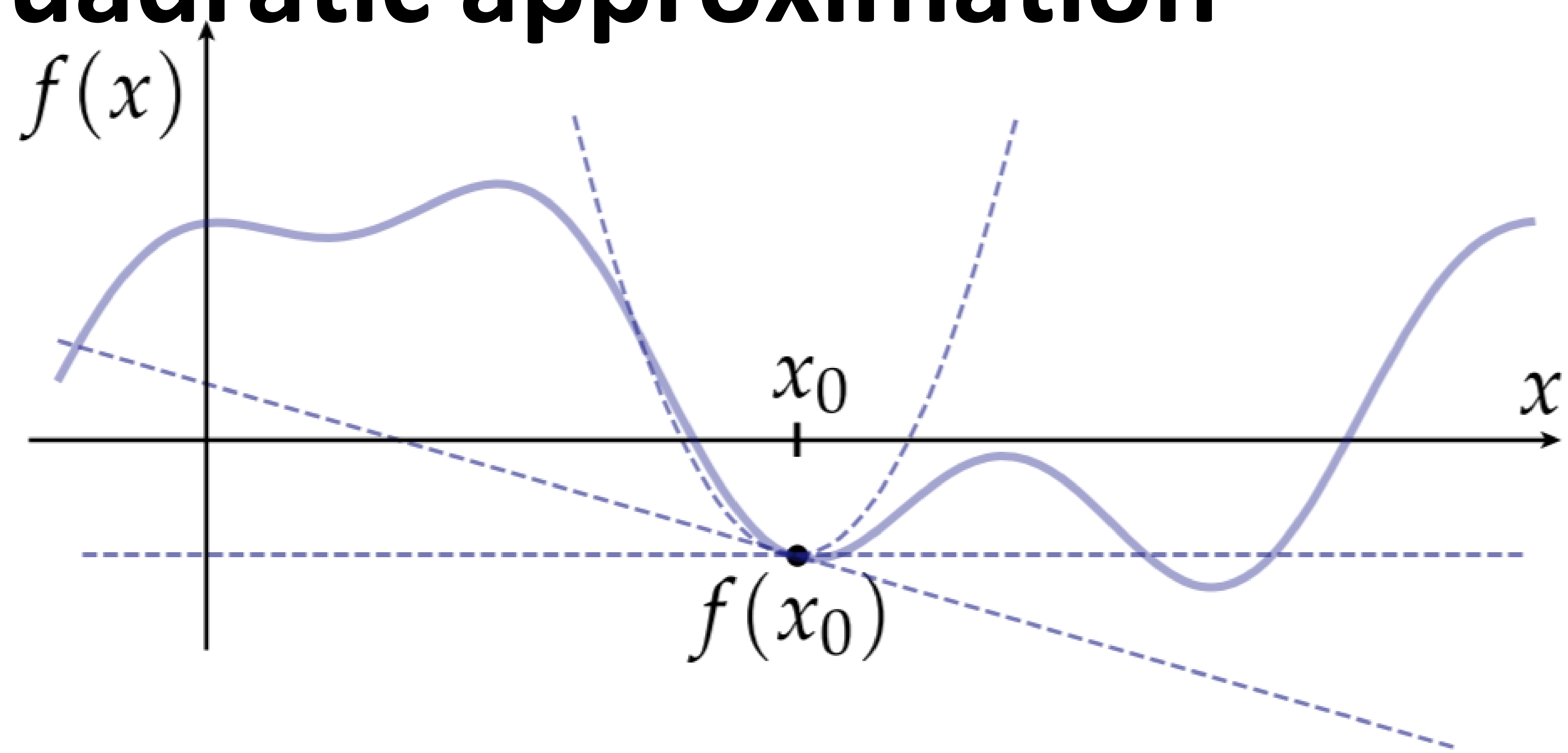
- **Jacobian of the gradient (matrix of second derivatives)**

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

- **Recall Taylor series**

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{(x-x_0)^2}{2!} f''(x_0) + \cdots$$

- **Gradient gives best linear approximation**
- **Hessian gives us best quadratic approximation**



Hessian and Optimality conditions

- **Optimality conditions for multivariate optimization?**

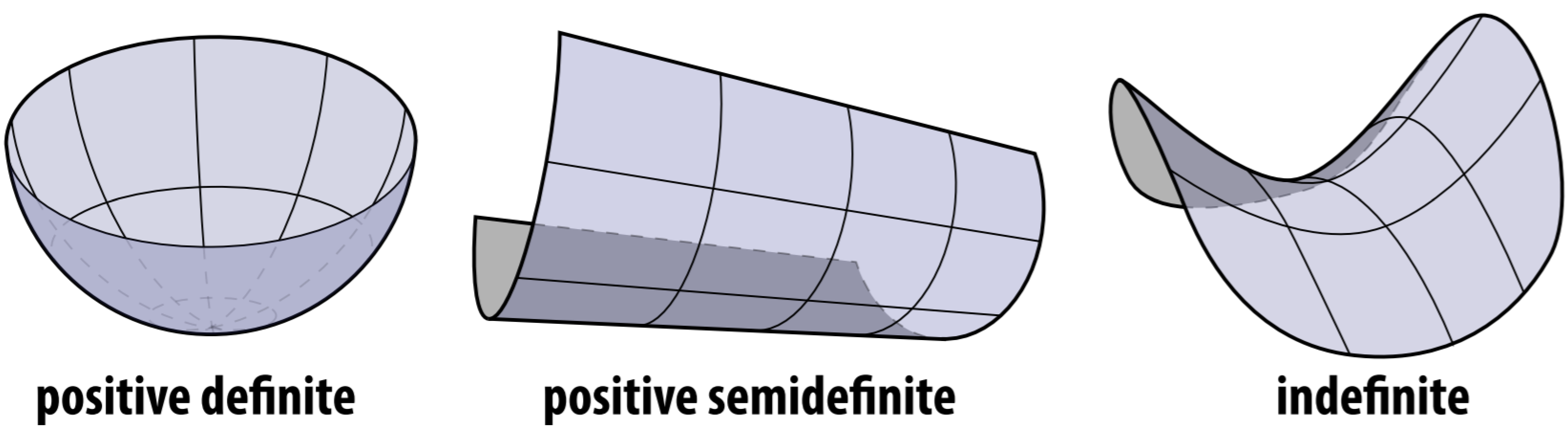
positive semidefinite (PSD)
($u^TAu \geq 0$ for all u)

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

1st order

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

2nd order



Gradients of Matrix-Valued Expressions

- **EXTREMELY useful to be able to differentiate matrix-valued expressions!**

For any two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and **symmetric** matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$:

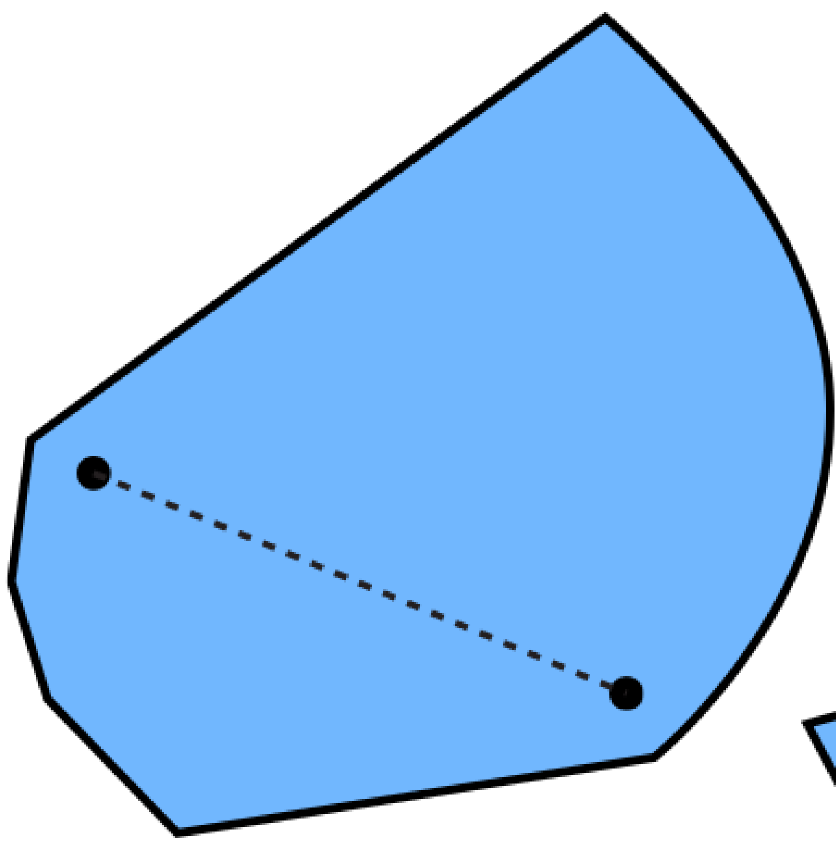
MATRIX DERIVATIVE	LOOKS LIKE
$\nabla_{\mathbf{x}}(\mathbf{x}^T\mathbf{y}) = \mathbf{y}$	$\frac{d}{dx}xy = y$
$\nabla_{\mathbf{x}}(\mathbf{x}^T\mathbf{x}) = 2\mathbf{x}$	$\frac{d}{dx}x^2 = 2x$
$\nabla_{\mathbf{x}}(\mathbf{x}^T A\mathbf{y}) = A\mathbf{y}$	$\frac{d}{dx}axy = ay$
$\nabla_{\mathbf{x}}(\mathbf{x}^T A\mathbf{x}) = 2A\mathbf{x}$	$\frac{d}{dx}ax^2 = 2ax$
$\ldots$	$\ldots$

Excellent resource: Petersen & Pedersen, "The Matrix Cookbook"

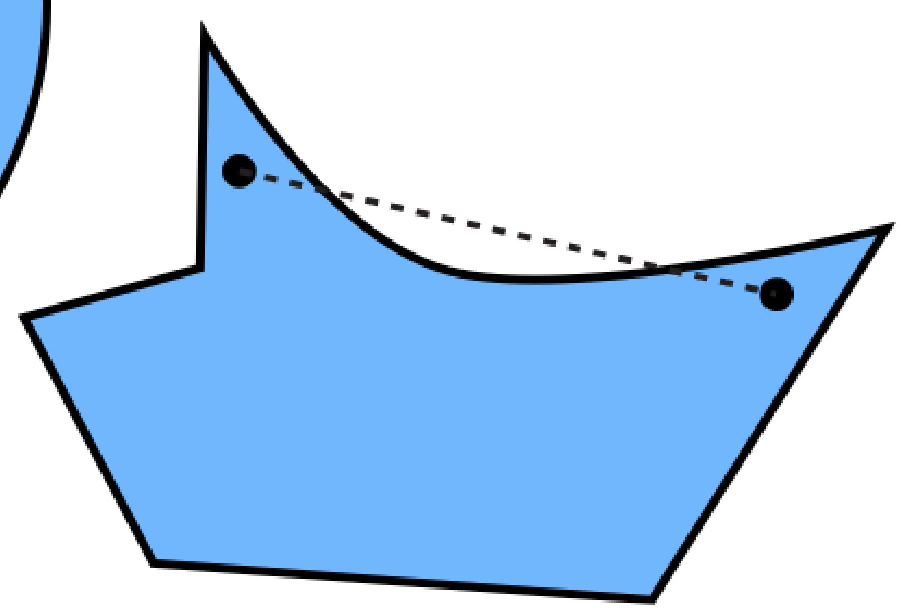
- **At least once in your life, work these out meticulously in coordinates!**
- **After that, http://www.matrixcalculus.org/**

Convex Optimization

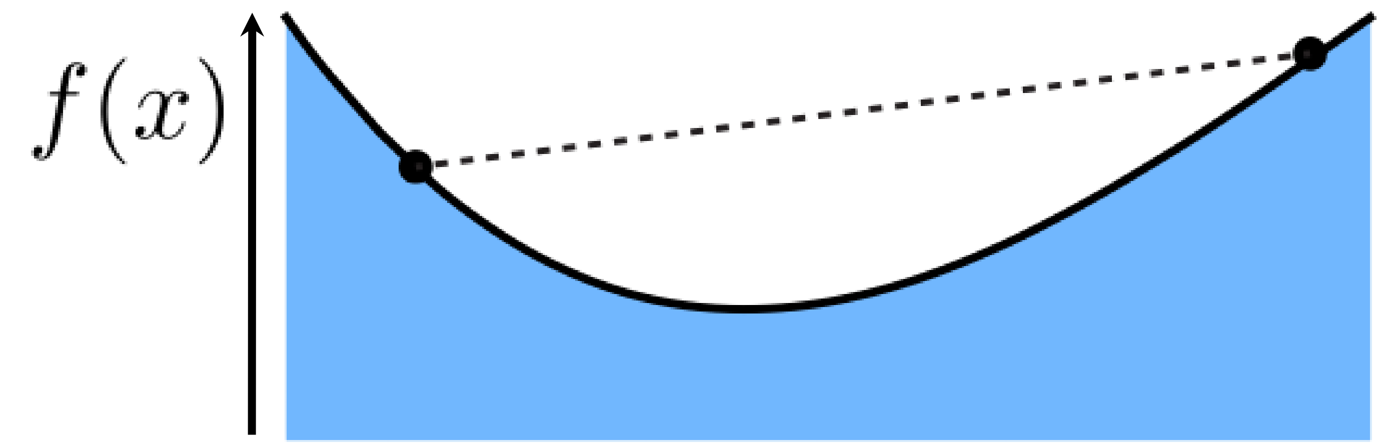
- Special class of problems that are almost always "easy" to solve (polynomial-time!)
- Problem is *convex* if it has a convex domain *and* convex objective



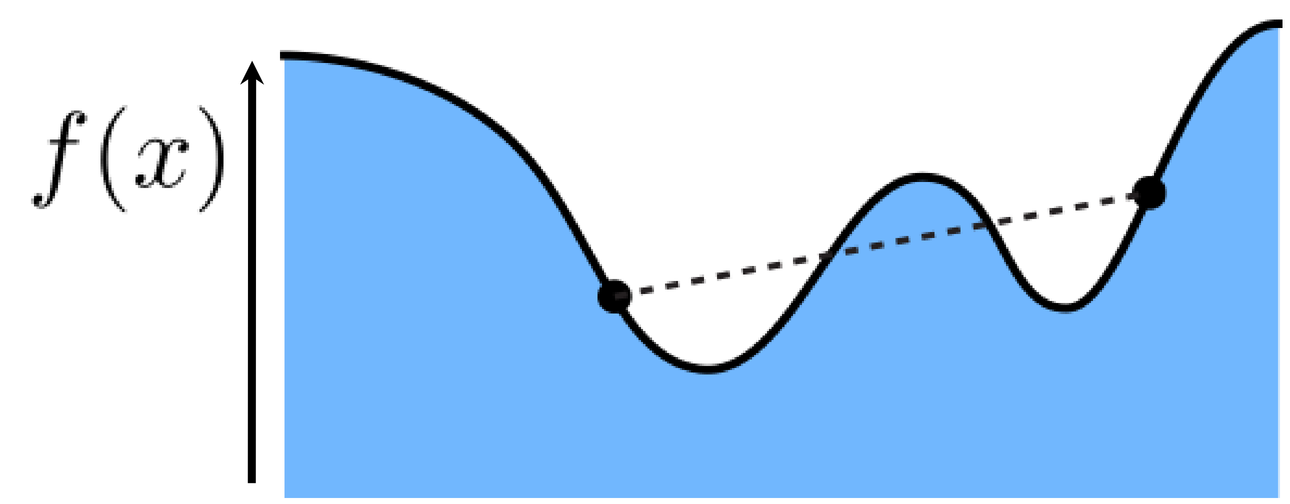
convex domain



noconvex domain



convex objective



nonconvex objective

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

Convex Quadratic Objectives & Linear Systems

- **Very important example: convex *quadratic* objective**
- **Can be expressed via positive-semidefinite (PSD) matrix:**

$$f_0(x) = \frac{1}{2}x^T A x - x^T b,\ A \succeq 0$$

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?

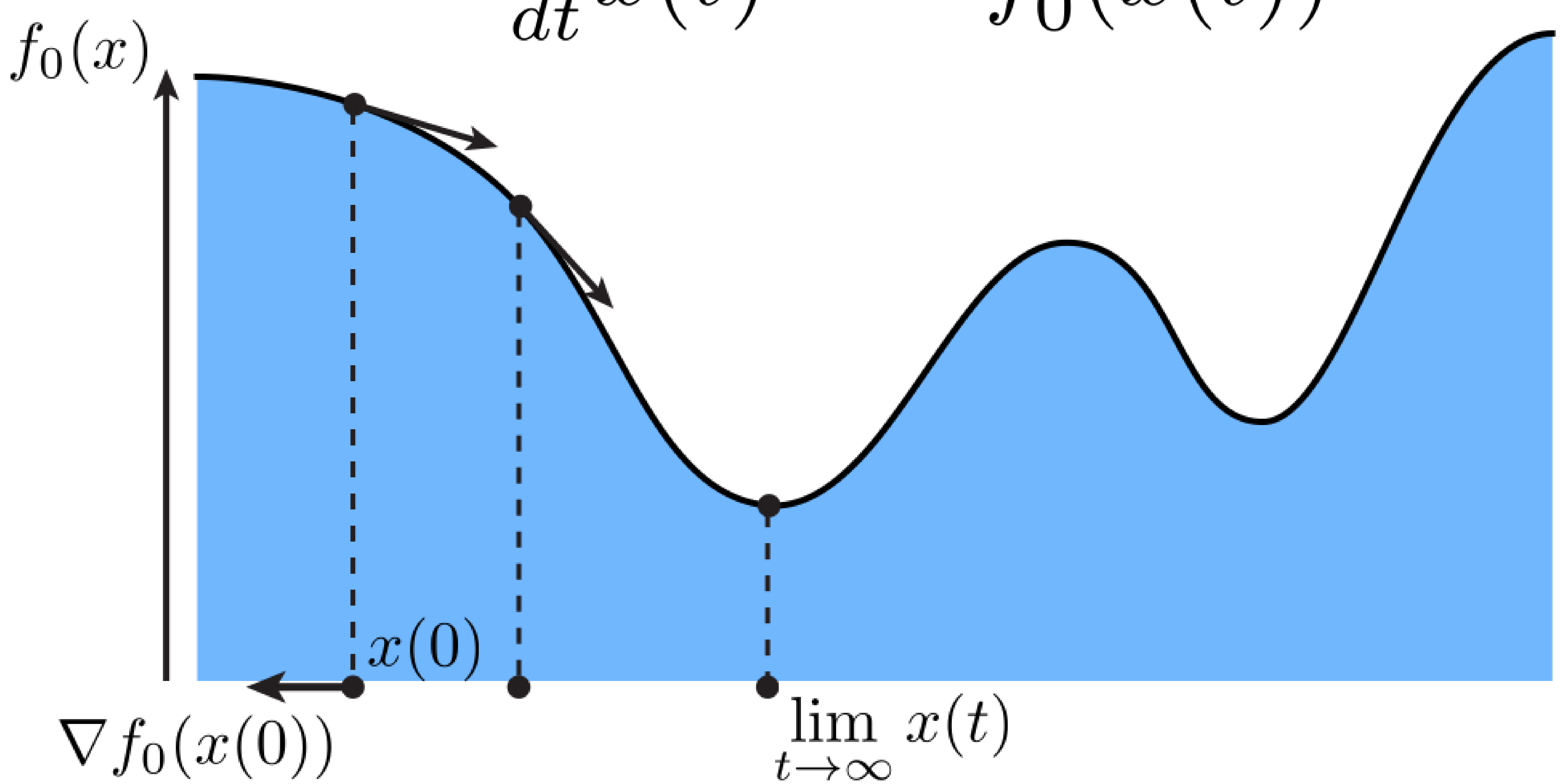
Descent Methods

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)**

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

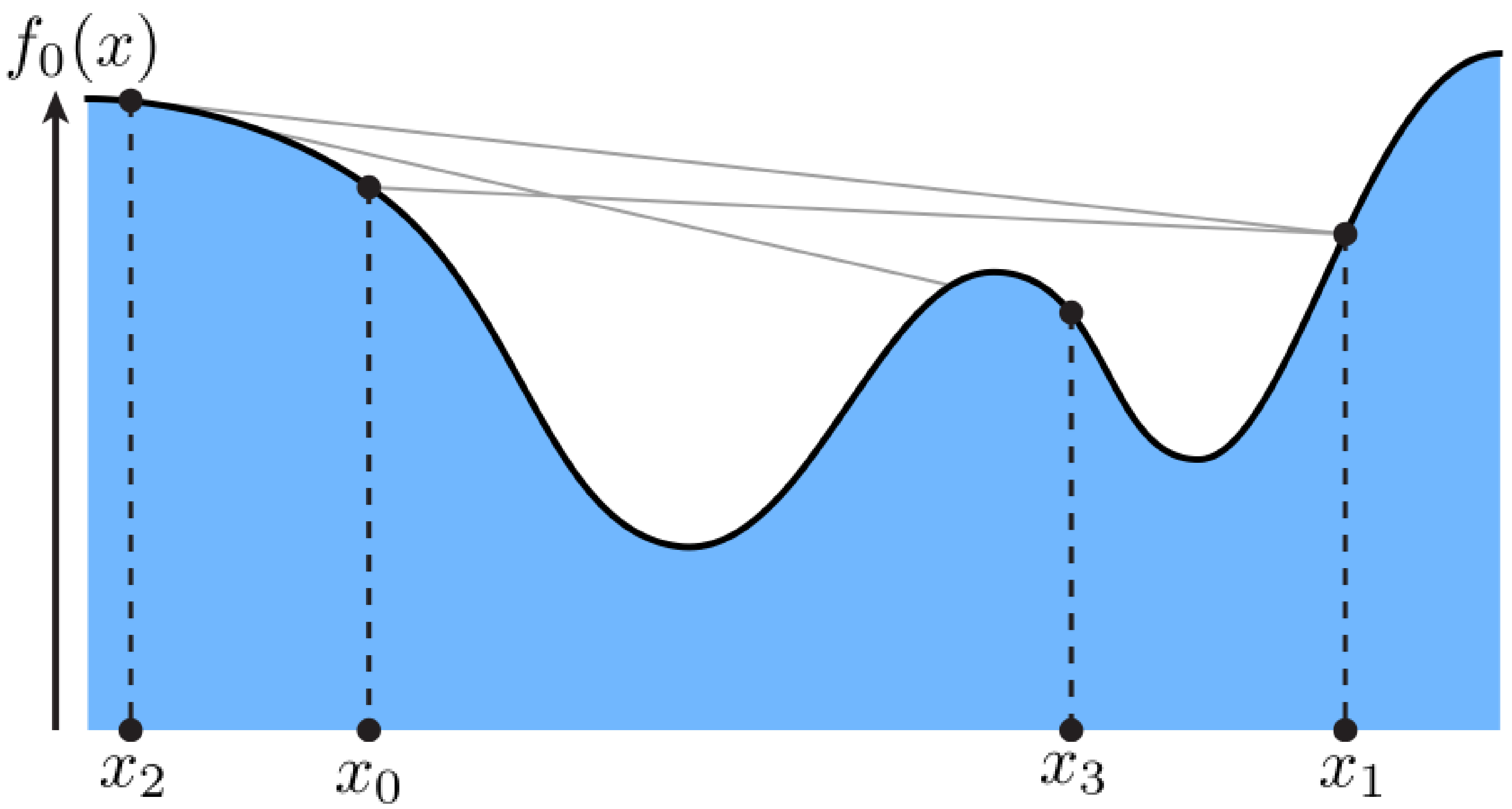


- **Do we always end up at a (global) minimum?**
- **How do we implement gradient descent in practice?**

Gradient Descent Algorithm (1D)

- **Simple update rule (go in direction that decreases objective):**

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

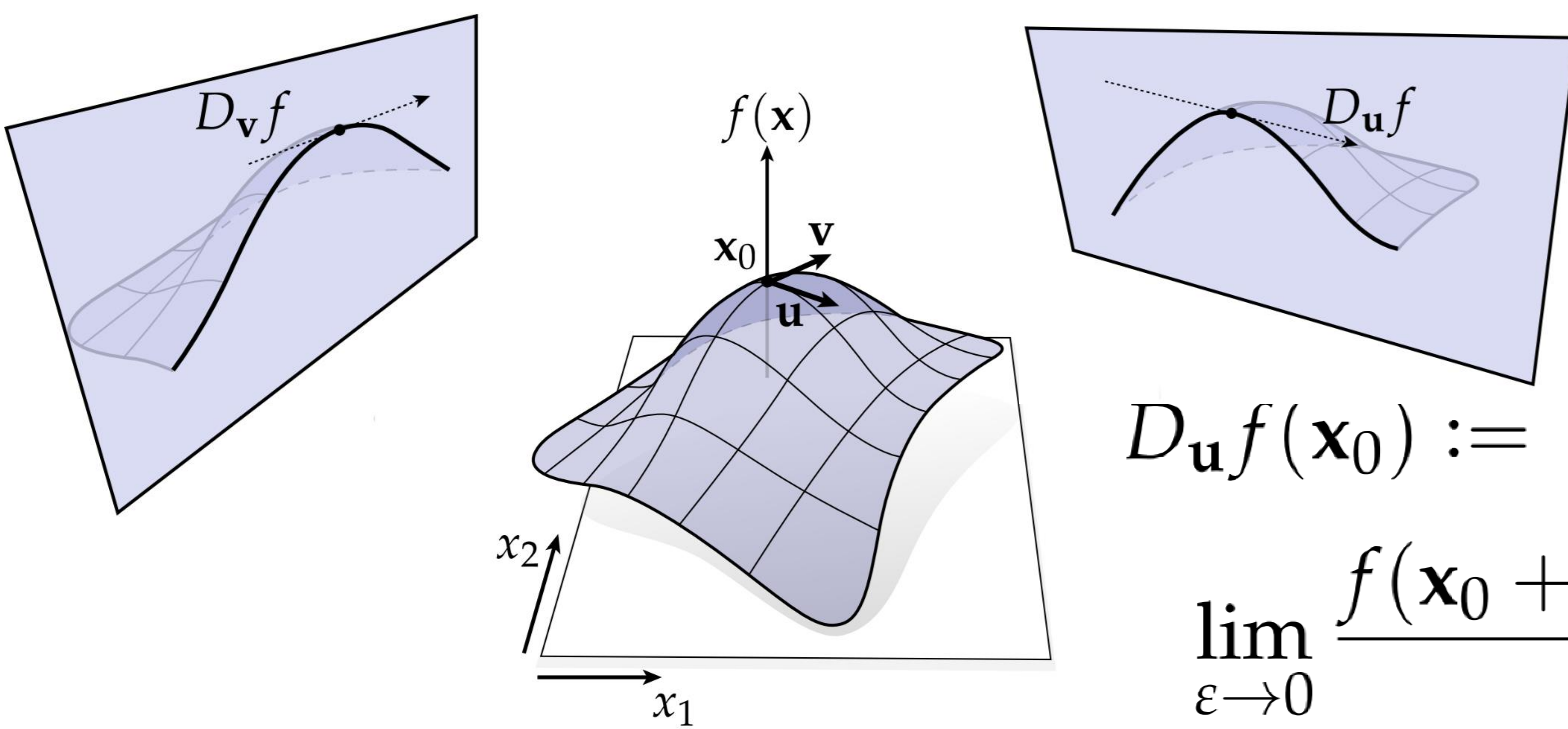


- **Q: How far should we go in that direction?**
- **If we're not careful, we'll be zipping all over the place!**
- **Basic idea: use *"step control"* to determine τ.**
- **Simple strategy: make τ *really small!***
- **Better idea: adaptive step size (e.g. bisection line search)**
- **A careful strategy (e.g., Armijo-Wolfe) can guarantee convergence at least to a *local* minimum.**

How do we go about optimizing a function of multiple variables?

Directional Derivative

- Suppose we have a function f(x1, x2)
  - Look at a slice through this function along some direction
  - Then apply the usual derivative concept (rise/run)!
  - This is called the directional derivative



take a small step along u

$$D_{\mathbf{u}} f(\mathbf{x}_0) := \lim_{\varepsilon \to 0} \frac{f(\mathbf{x}_0 + \varepsilon \mathbf{u}) - f(\mathbf{x}_0)}{\varepsilon}$$

Directional Derivative

- **Starting from Taylor's series**

$$f(x_0+\Delta x) \approx f(x_0) + \Delta x^T \nabla \mathrm{f}(\mathrm{x}_0) + \frac{1}{2}\Delta x^T \nabla^2 \mathrm{f}(\mathrm{x}_0)\Delta x$$

easy to see that

take a small step along u

$$D_{\mathbf{u}} f(\mathbf{x}_0) := \lim_{\varepsilon \to 0} \frac{f(\mathbf{x}_0 + \varepsilon \mathbf{u}) - f(\mathbf{x}_0)}{\varepsilon} = \frac{f(x_0) + \varepsilon \boldsymbol{u}^t \nabla f(\mathrm{x}_0) - f(x_0)}{\varepsilon}$$

$$D_{\boldsymbol{u}} f = \boldsymbol{u}^T \nabla f$$

Q: What does this mean?

Directional Derivative and the Gradient

- **Given a multivariate function $f(x)$, gradient assigns a vector $\nabla f(x)$ at each point**

Directional Derivative and the Gradient

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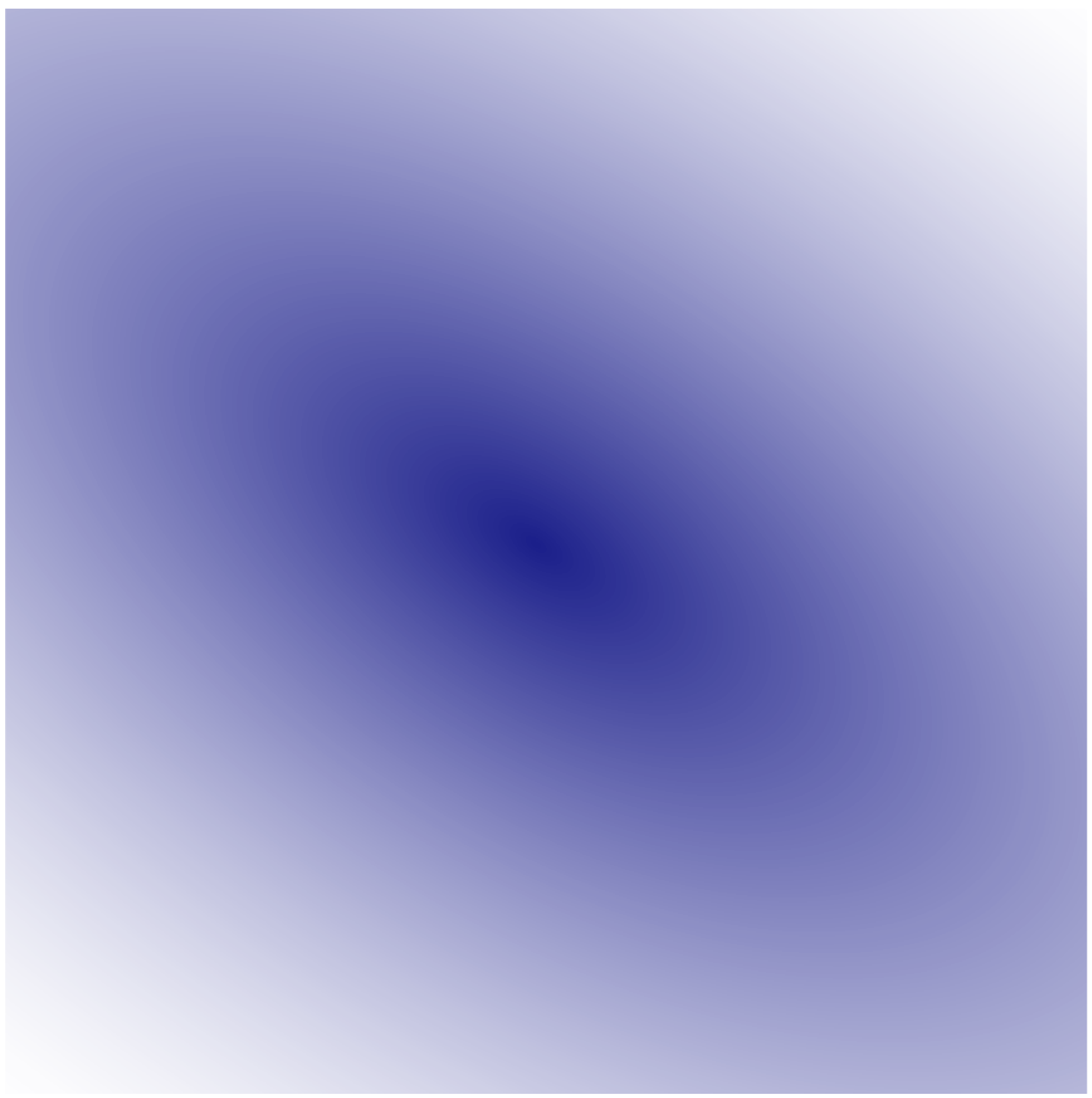
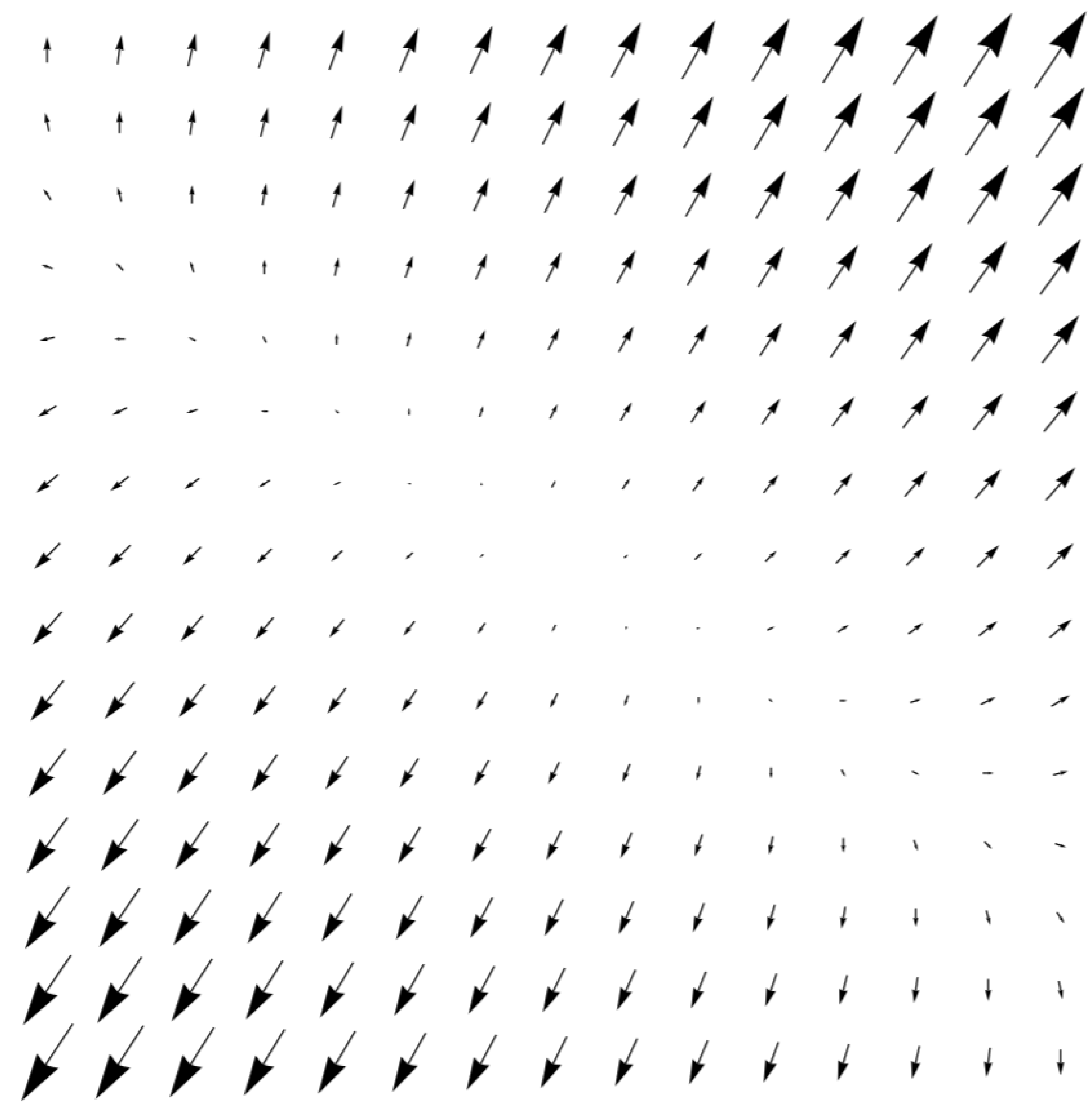


$f(\mathbf{x})$



$\nabla f(\mathbf{x})$

Gradient in coordinates

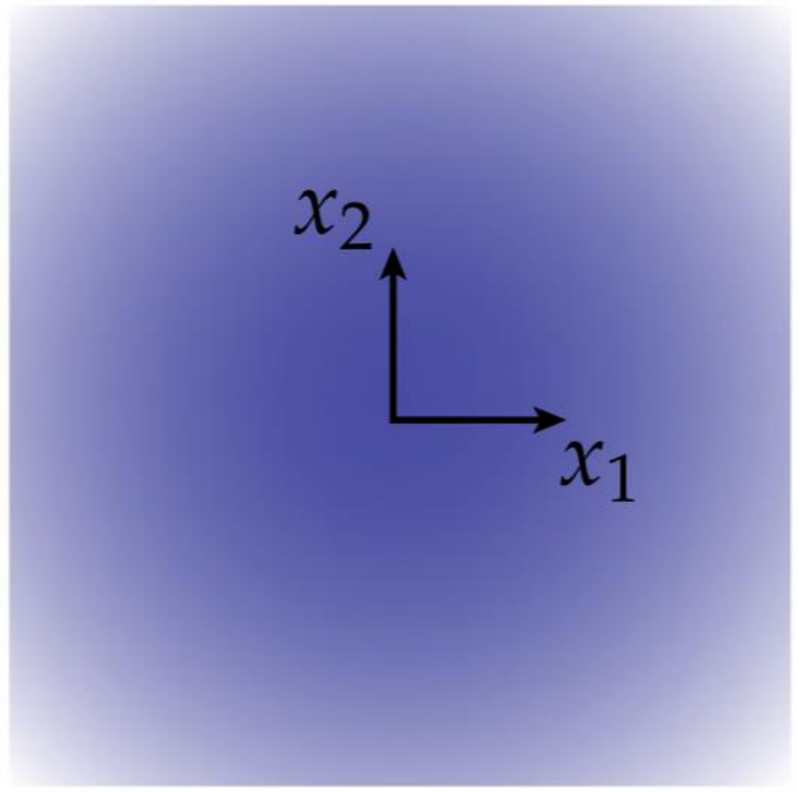
- **Most familiar definition: list of partial derivatives**

$$f(\mathbf{x}) := x_1^2 + x_2^2$$

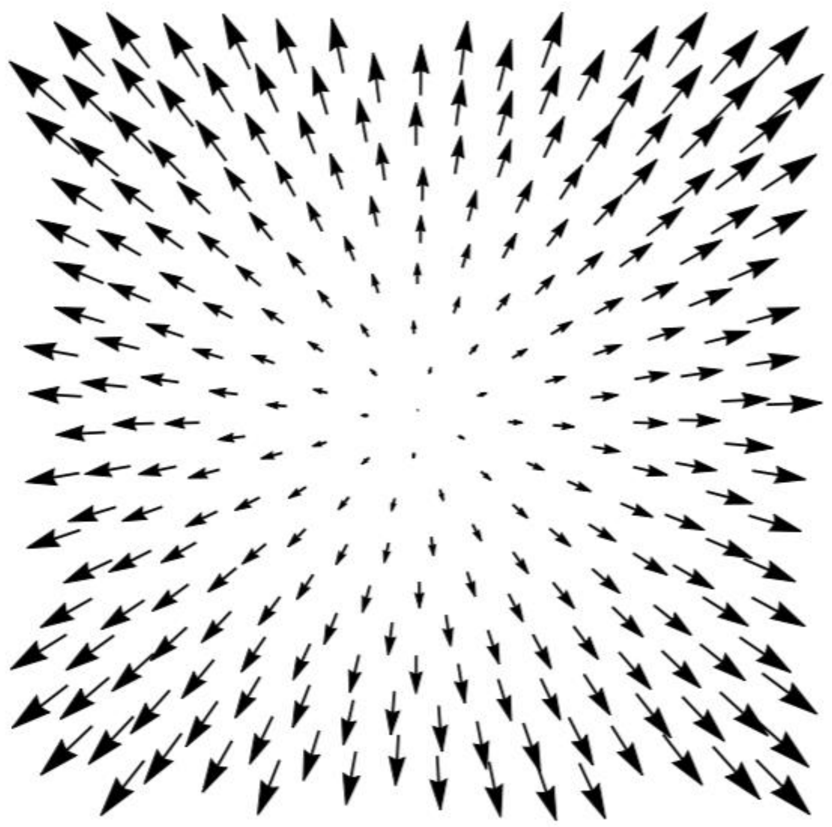
$$\frac{\partial f}{\partial x_1} = \frac{\partial}{\partial x_1} x_1^2 + \frac{\partial}{\partial x_1} x_2^2 = 2x_1 + 0$$

$$\frac{\partial f}{\partial x_2} = \frac{\partial}{\partial x_2} x_1^2 + \frac{\partial}{\partial x_2} x_2^2 = 0 + 2x_2$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} = 2\mathbf{x}$$



$f(\mathbf{x})$



$\nabla f(\mathbf{x})$

Directional Derivative and the Gradient

- **Given a multivariate function $f(x)$, gradient assigns a vector $\nabla f(x)$ at each point**

- **Inner product between gradient and any unit vector gives directional derivative "along that direction"**

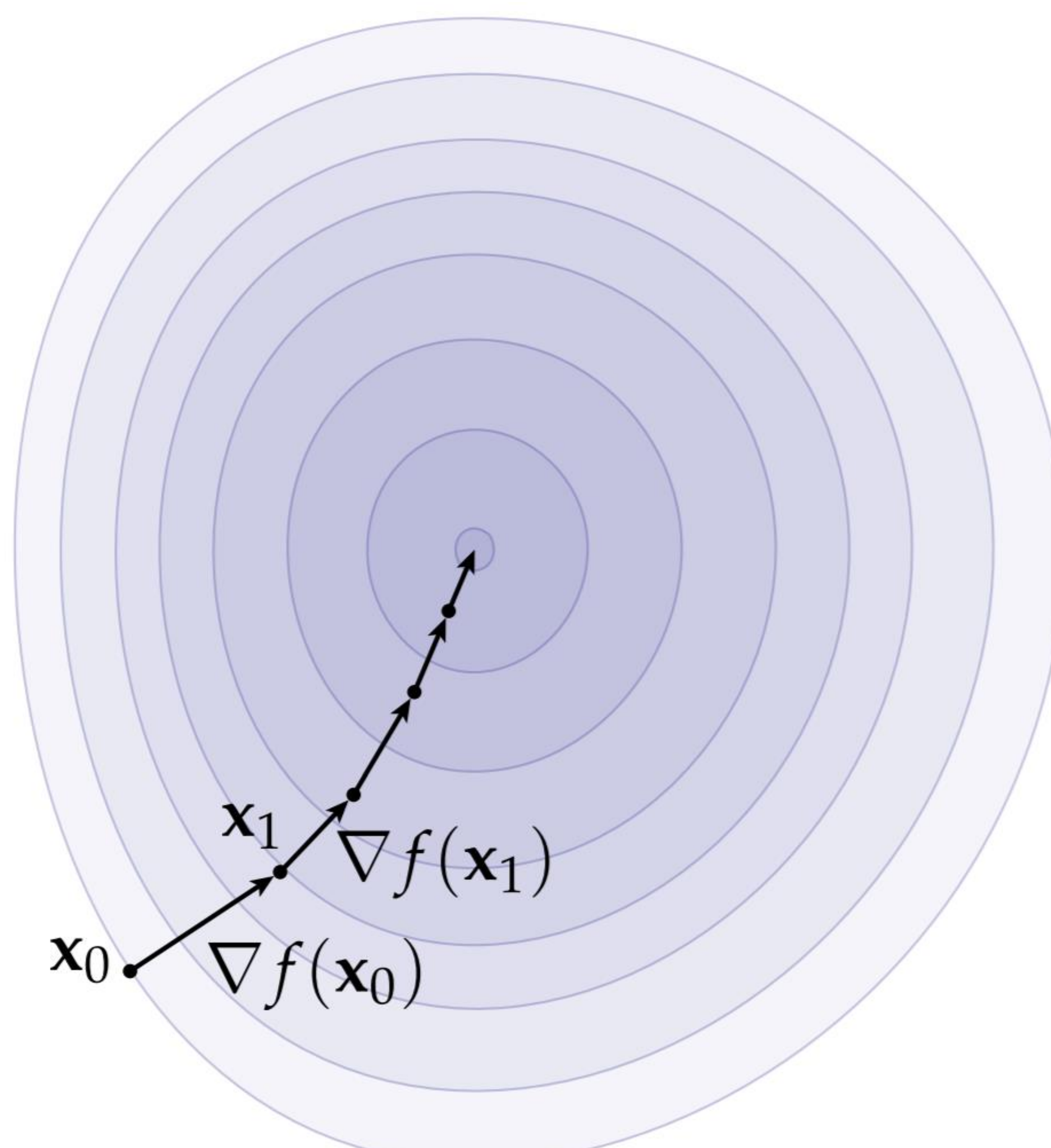
$$D_{\boldsymbol{u}} f = \boldsymbol{u}^T \nabla f$$

- **Out of all possible (unit vectors) directions in x, which is the one along which the function increases most?**

- **Gradient points in direction of steepest ascent; its magnitude tells you how much the function is changing in that direction.**

The Gradient

- **Function value**
  - **gets largest if we move in direction of gradient**
  - **doesn't change if we move orthogonally (gradient is perpendicular to isolines)**
  - **decreases *fastest* if we move exactly in opposite direction**

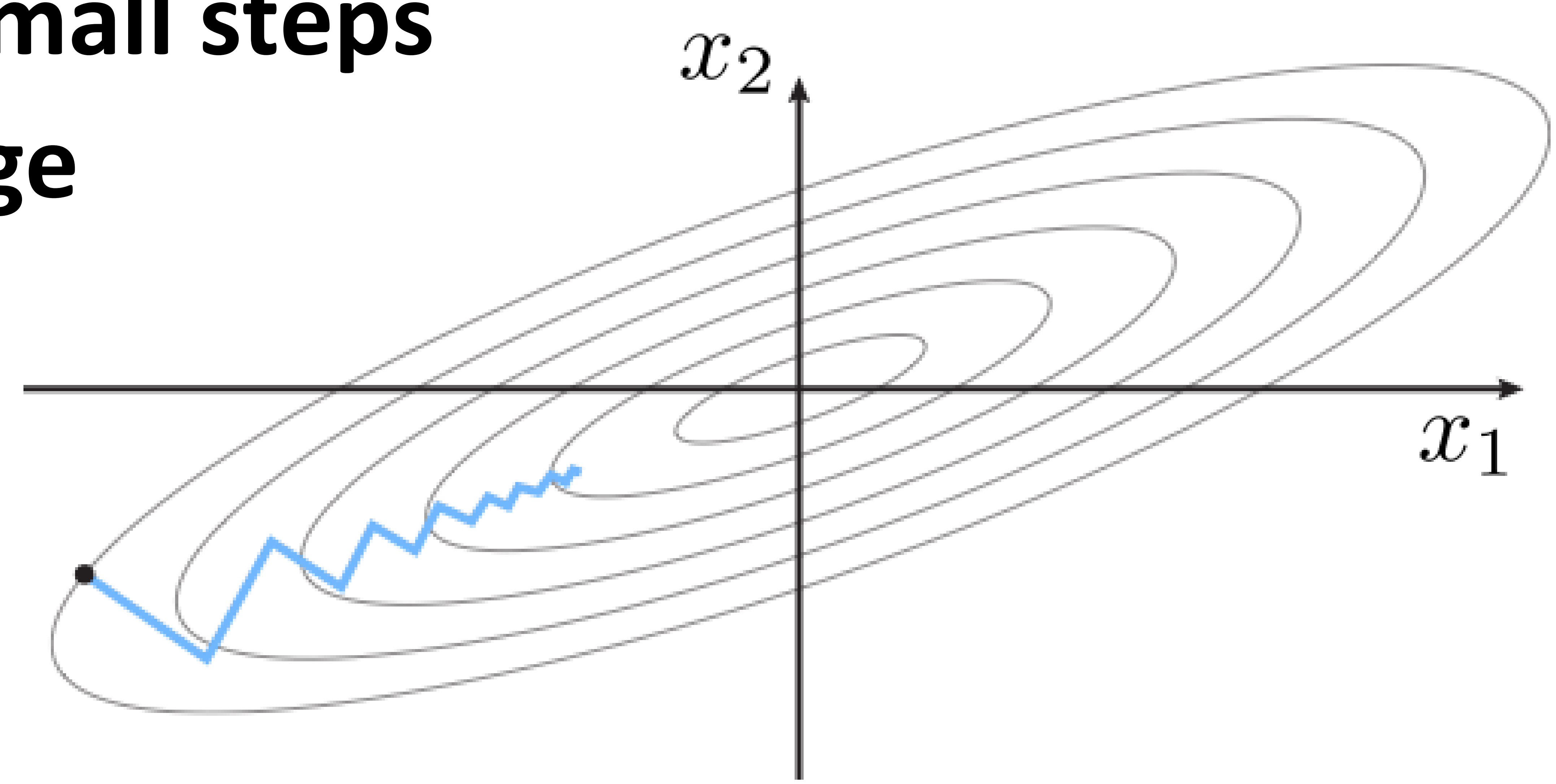


Gradient Descent Algorithm (nD)

Q: What's the corresponding update in higher dimensions?

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

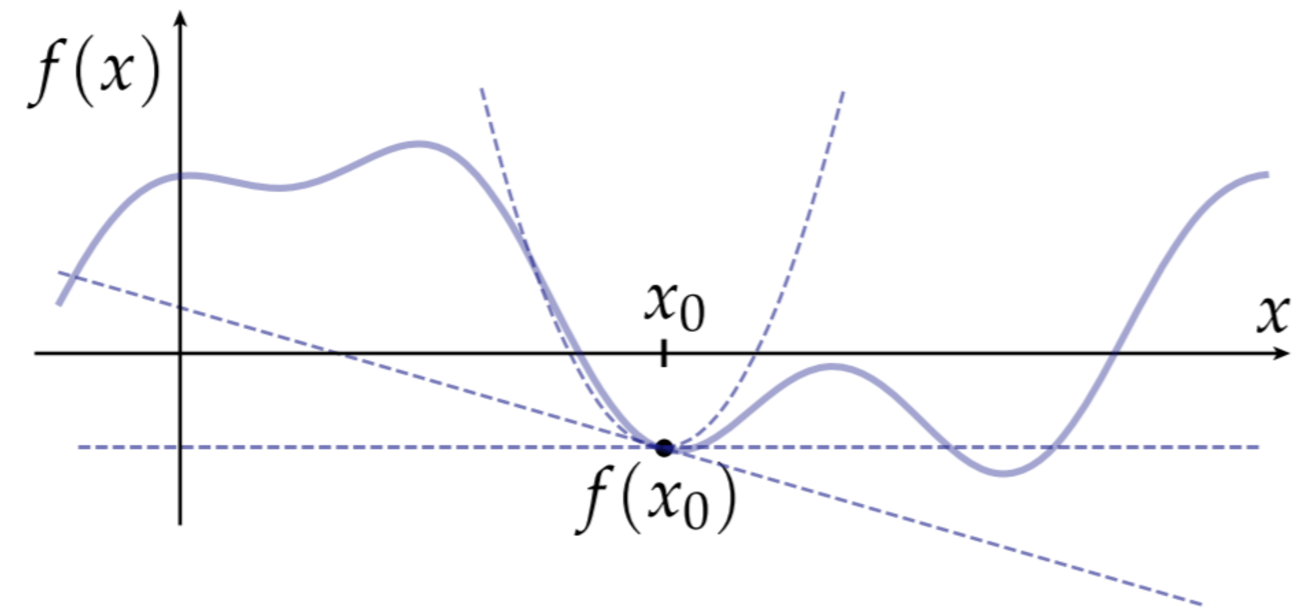
- **Basic challenge in nD:**
  - **solution can "oscillate"**
  - **takes many, many small steps**
  - **very slow to converge**



Higher Order Descent

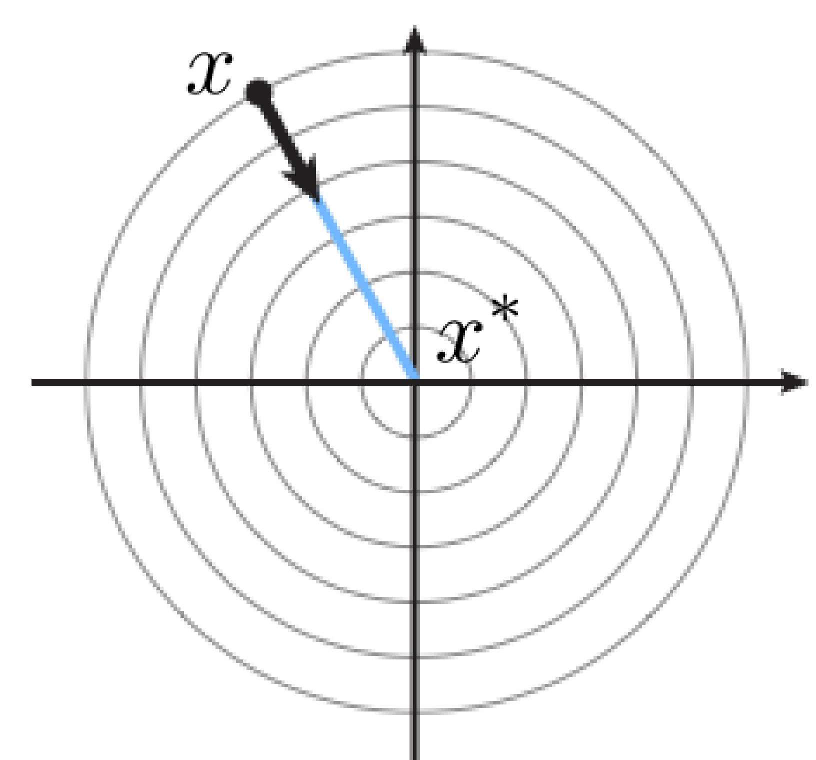
- **Newton's method:**
  - **General idea: "pretend" the function is quadratic, solve, and repeat.**

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



- **Another way to think about it: apply a coordinate transformation so that the local energy landscape looks more like a "round bowl"**

Gradient now points directly towards stationary point



Newton's method and beyond…

- Great for convex problems
- For nonconvex problems, need to be more careful
- In general, nonconvex optimization is a *BLACK ART*
- That you should aim to master…

Do you know?

- What might happen if the Hessian is not PSD?
- How to check derivatives with FD?
- What regularization means?
  - Eigenvalue picture
  - The objective it corresponds to
- Why Gauss-Newton for non-linear least square problems is always PSD?
- Why linesearch is needed, and how to implement it?