Optimization

CMPUT 267: Basics of Machine Learning

Textbook §4.1-4.4

Comments

- Assignment 1 due this week
- Hope you enjoyed doing the thought questions
- Quiz will be on eClass (remote), during class time (synchronous)
- Please ask each other questions on Discord
    - If you are not sure you are allowed, err on the side of asking
    - Just don’t post solutions, instead questions
    - You can post a chunk of your code and ask for comments
- Any questions?

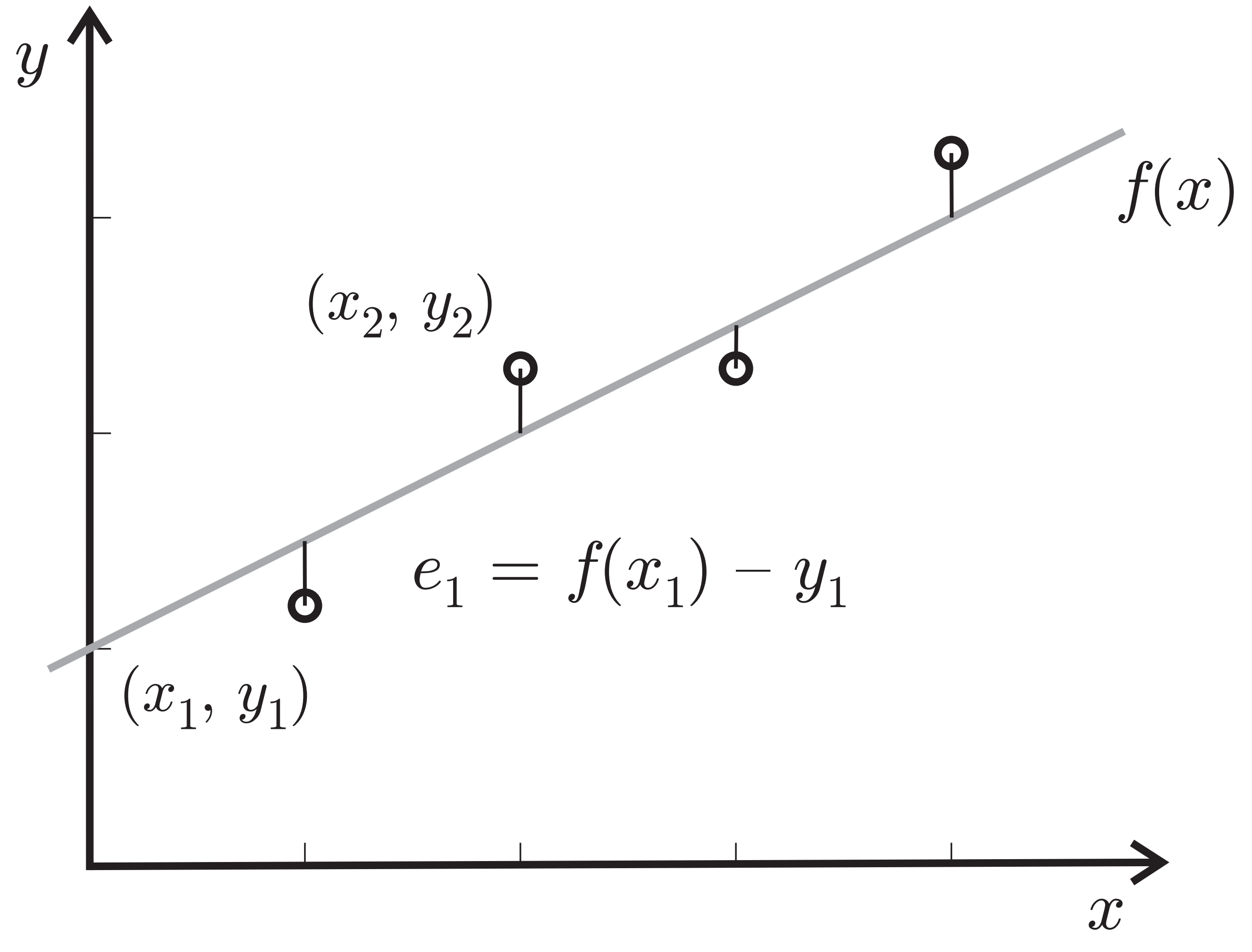
Optimization

We often want to find the argument w^* that **minimizes** an **objective function** c

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} c(\mathbf{w})$$

Example: Using linear regression to fit a dataset $\{(x_i, y_i)\}_{i=1}^{n}$

- Estimate the targets by $\hat{y} = f(x) = w_0 + w_1 x$
- Each vector $\mathbf{w}$ specifies a particular f
- Objective is the **total error** $c(\mathbf{w}) = \sum_{i=1}^{n} (f(x_i) - y_i)^2$



Exercise: Making your own optimization algorithm

- Imagine I told you that you need to find

$$\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathbb{R}^d} c(\mathbf{w})$$

- Pretend you have never heard of gradient descent. What algorithm might you design to find this?

- Now what if I told you that $w \in \mathscr{W} = \{1,2,3,...,1000\}$. Now how would you solve

$$\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathscr{W}} c(\mathbf{w})$$

Optimization Properties

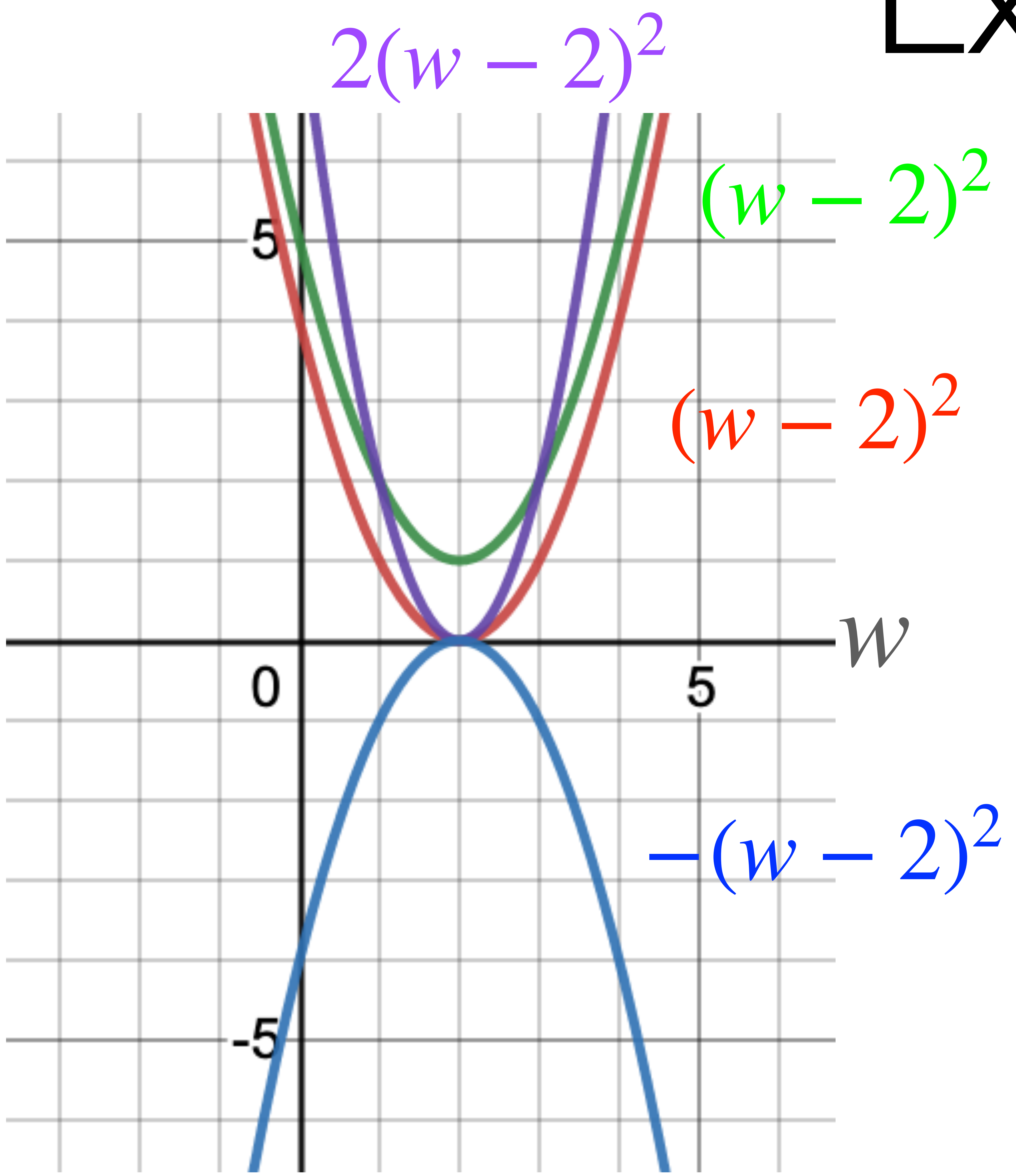
1. **Maximizing** $c(w)$ is the same as minimizing $-c(w)$:

$$\arg\max_{w} c(w) = \arg\min_{w} - c(w)$$

2. **Equivalence under constant shifts:** Adding, subtracting, or multiplying by a positive constant **does not change** the minimizer of a function:

$$\arg\min_{w} c(w) = \arg\min_{w} c(w)+k = \arg\min_{w} c(w)-k = \arg\min_{w} kc(w) \quad \forall k \in \mathbb{R}^{+}$$

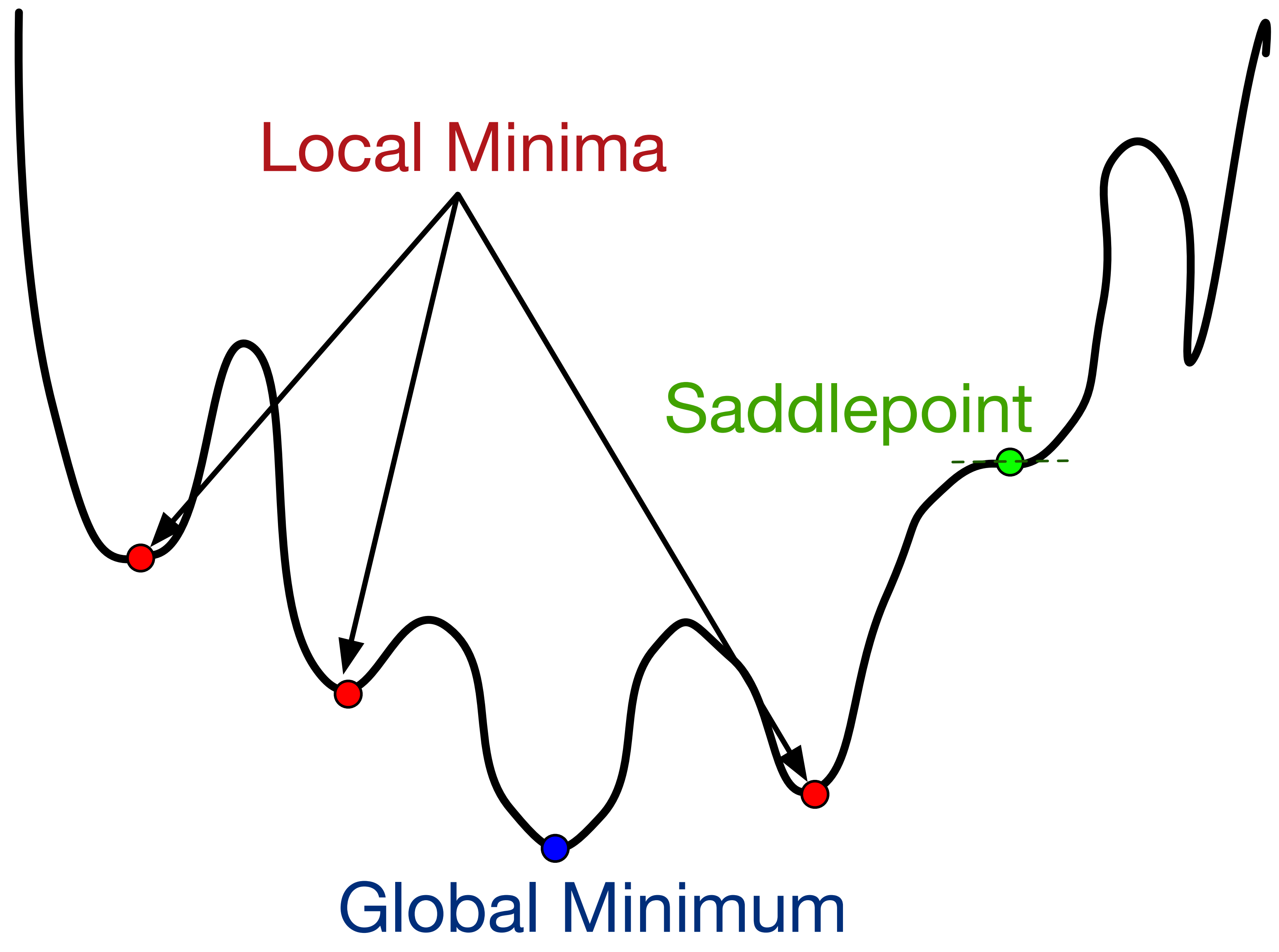
Example



$$\arg\min_{w\in\mathbb{R}} (w-2)^2$$
$$= \arg\min_{w\in\mathbb{R}} 2(w-2)^2$$
$$= \arg\min_{w\in\mathbb{R}} (w-2)^2 + 1$$
$$= \arg\max_{w\in\mathbb{R}} -(w-2)^2$$
$$= 2$$

Stationary Points

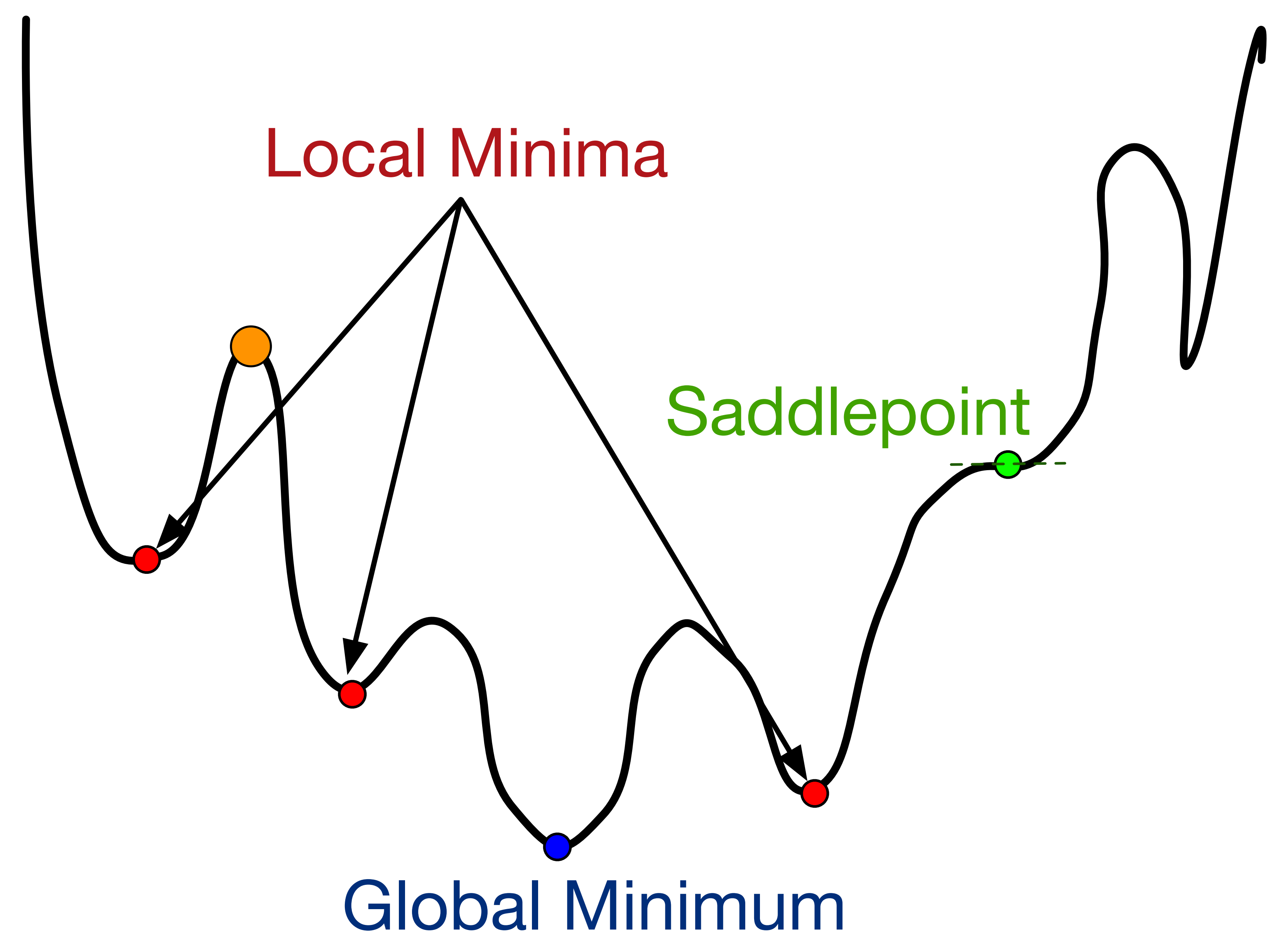
- Every minimum of an everywhere-differentiable function $c(w)$ **must** occur at a **stationary point**: A point at which $c'(w) = 0$
- However, not every stationary point is a minimum
- Every stationary point is either:
  - A **local minimum**
  - A **local maximum**
  - A **saddlepoint**
- The **global minimum** is either a local minimum (or a boundary point)



Let's assume for now that w is unconstrained (i.e, $w \in \mathbb{R}$ rather than $w \geq 0$ or $w \in [0,1]$)

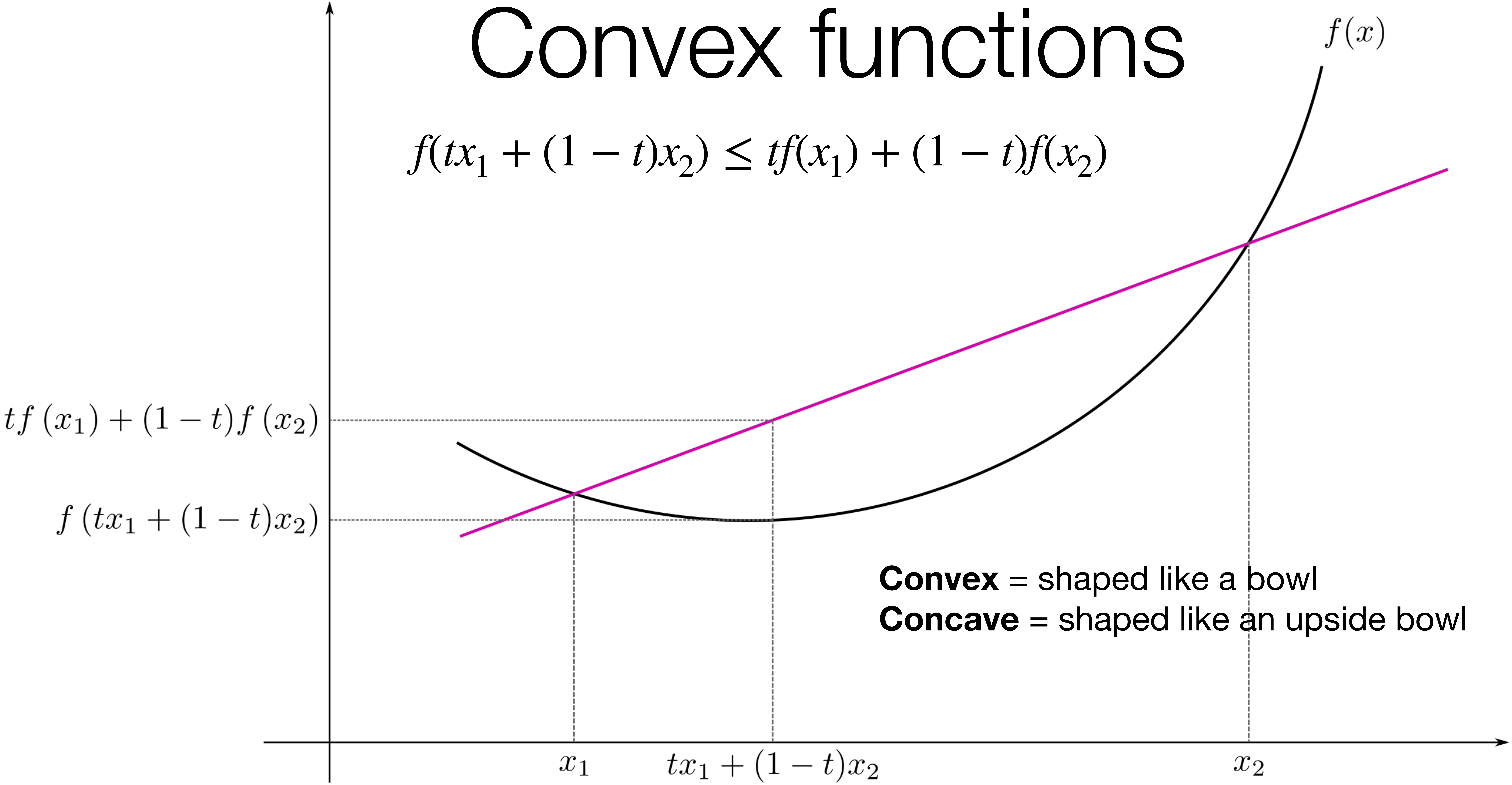
Identifying the type of the stationary point

- If function curved upwards (**convex**) locally, then **local minimum**



Convex functions

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

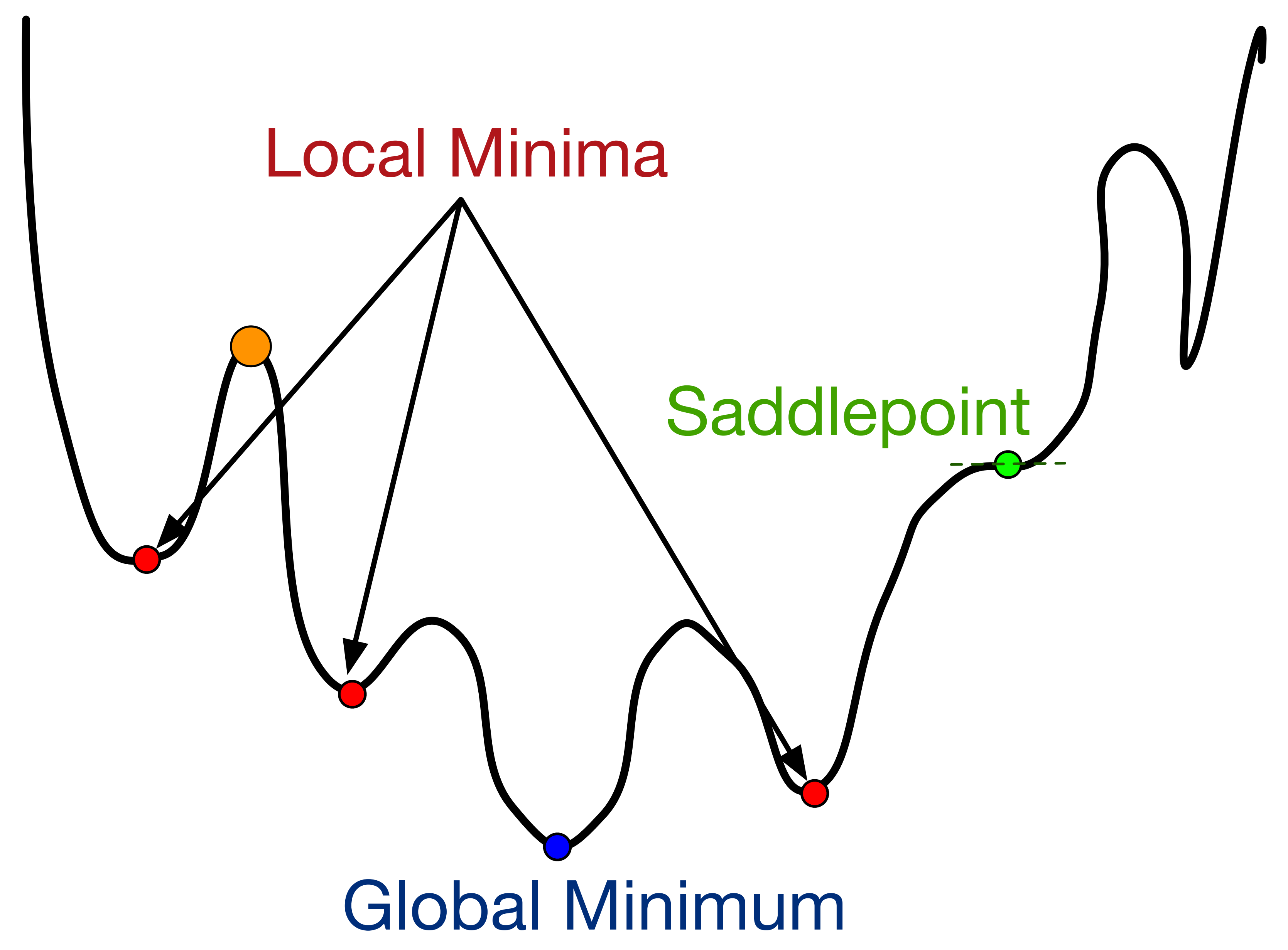


Convex = shaped like a bowl
Concave = shaped like an upside bowl

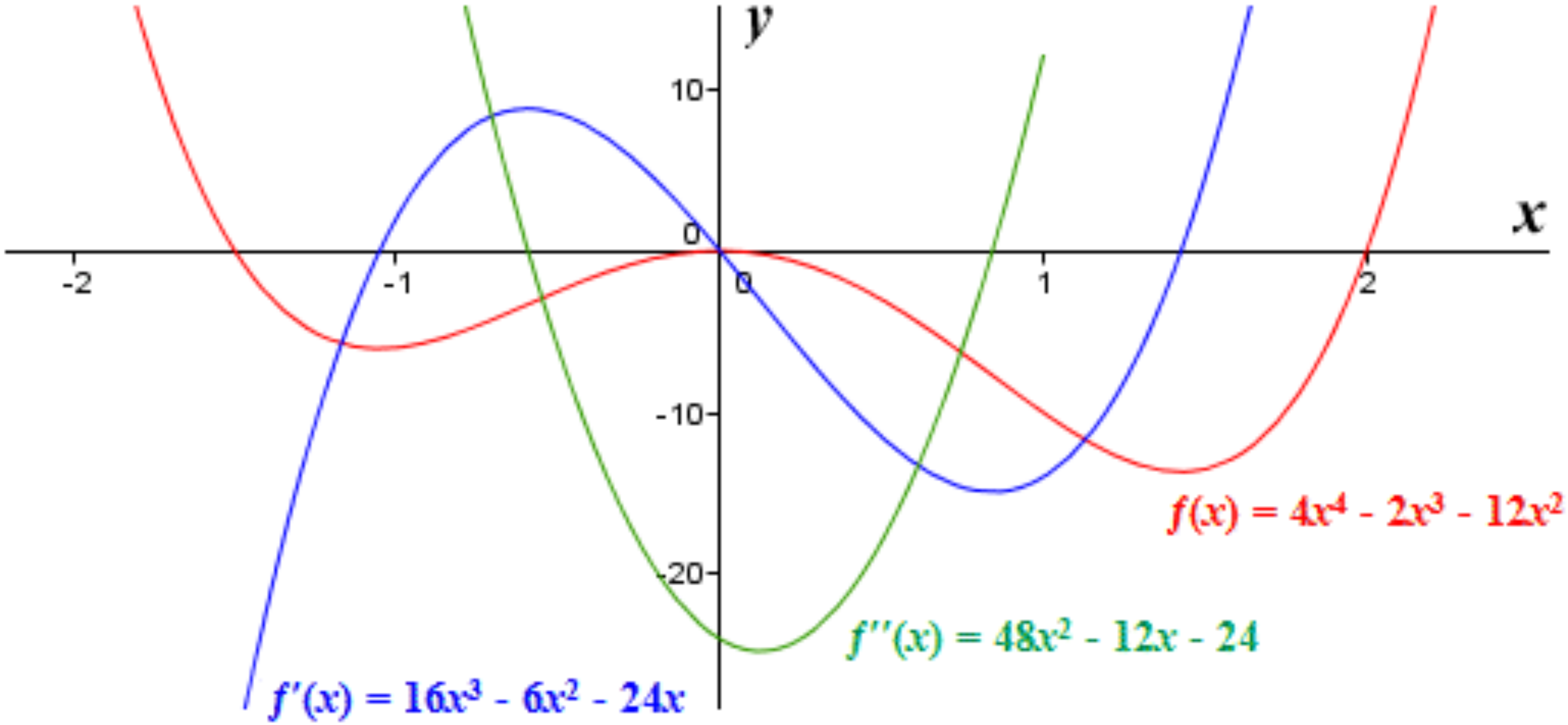
* from Wikipedia

Identifying the type of the stationary point

- If function curved upwards (**convex**) locally, then **local minimum**
- If function curved downwards (**concave**) locally, then **local maximum**
- If function **flat** locally, then might be a **saddlepoint** but could also be a local min or local max
- Locally, cannot distinguish between local min and global min (its a global property of the surface)

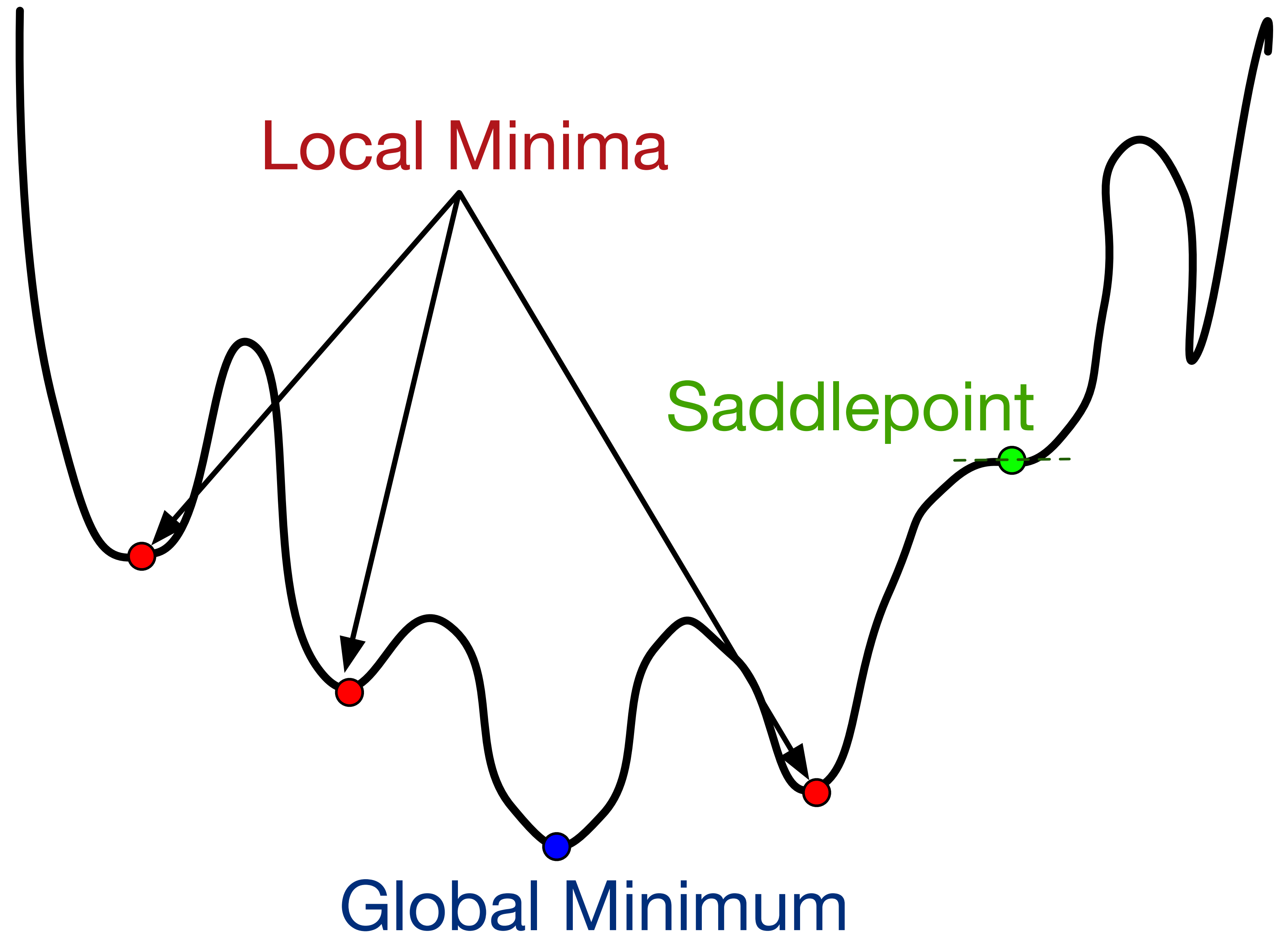


Second derivative reflects curvature



Second derivative test

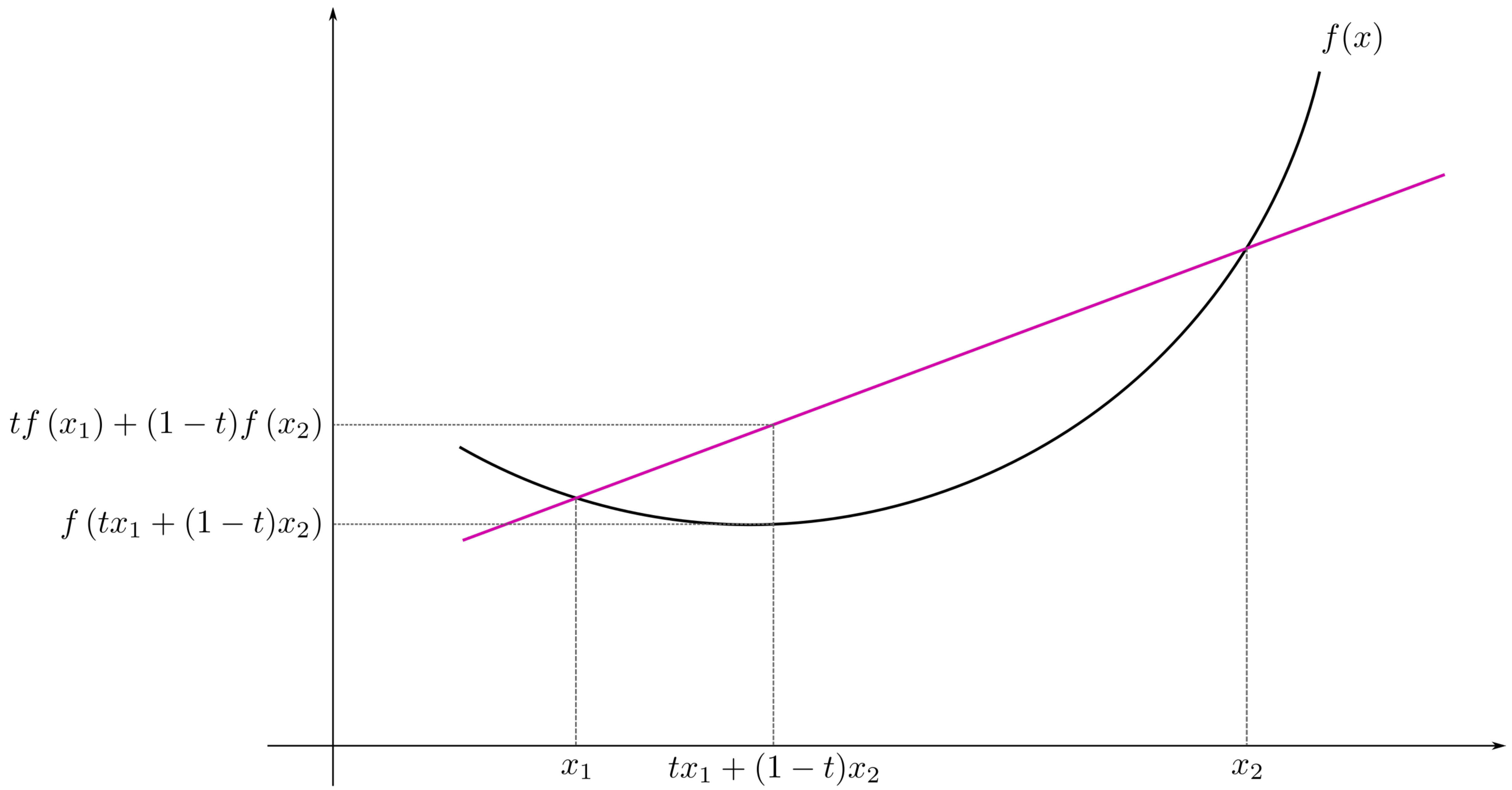
1. If $c''(w_0) > 0$ then w_0 is a local minimum.
2. If $c''(w_0) < 0$ then w_0 is a local maximum.
3. If $c''(w_0) = 0$ then the test is inconclusive: we cannot say which type of stationary point we have and it could be any of the three.



Testing optimality without the second derivative test

Convex functions have a **global** minimum at **every** stationary point

$$c \text{ is convex} \iff c(t\mathbf{w}_1 + (1-t)\mathbf{w}_2) \leq tc(\mathbf{w}_1) + (1-t)c(\mathbf{w}_2)$$



Procedure

- Find a stationary point, namely w_0 such that $c'(w_0) = 0$
  - Sometimes we can do this analytically (closed form solution, namely an explicit formula for w_0)
- Reason about if it is optimal
  - Check if your function is convex
  - If you have only one stationary point and it is a local minimum, then it is a global minimum
  - Otherwise, if second derivate test says its a local min, can only say that

Exercise

- Find the solution to the optimization problem $\min_{w \in \mathbb{R}} (w - 2)^2 + (w - 3)^2$
- Recall that the procedure is:
  - 1. Find a stationary point, namely w_0 such that $c'(w_0) = 0$
  - 2. Do the second derivative test (or reason about if this function is convex)

Exercise: Prove equivalence under constant shifts

Equivalence under constant shifts: Adding, subtracting, or multiplying by a positive constant **does not change** the minimizer of a function:

$$\arg\min_w c(w) = \arg\min_w c(w) + k = \arg\min_w c(w) - k = \arg\min_w kc(w) \quad \forall k \in \mathbb{R}^+$$

Show that all of these have the same set of stationary points,
namely points w where c'(w) = 0

Numerical Optimization

- We will *almost never* be able to **analytically** compute the minimum of the functions that we want to optimize
  - (Linear regression is an important exception)
- Instead, we must try to find the minimum **numerically**
- Main techniques: First-order and second-order **gradient descent**

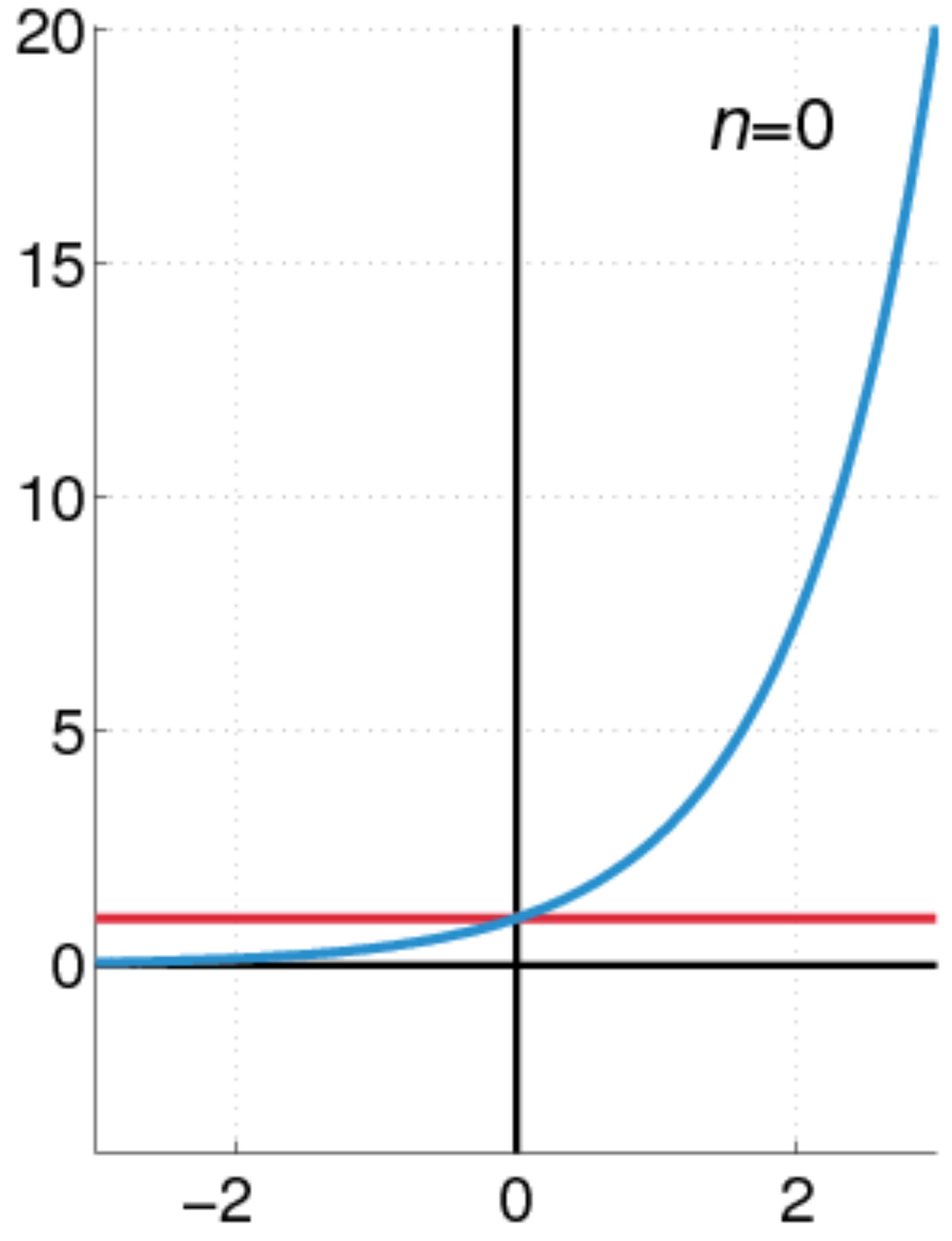
Taylor Series

Definition: A **Taylor series** is a way of approximating a function c in a small neighbourhood around a point a:

$$c(w) \approx c(a) + c'(a)(w-a) + \frac{c''(a)}{2}(w-a)^2 + \cdots + \frac{c^{(k)}(a)}{k!}(w-a)^k$$

$$= c(a) + \sum_{i=1}^{k} \frac{c^{(i)}(a)}{i!}(w-a)^i$$

Taylor Series Visualization

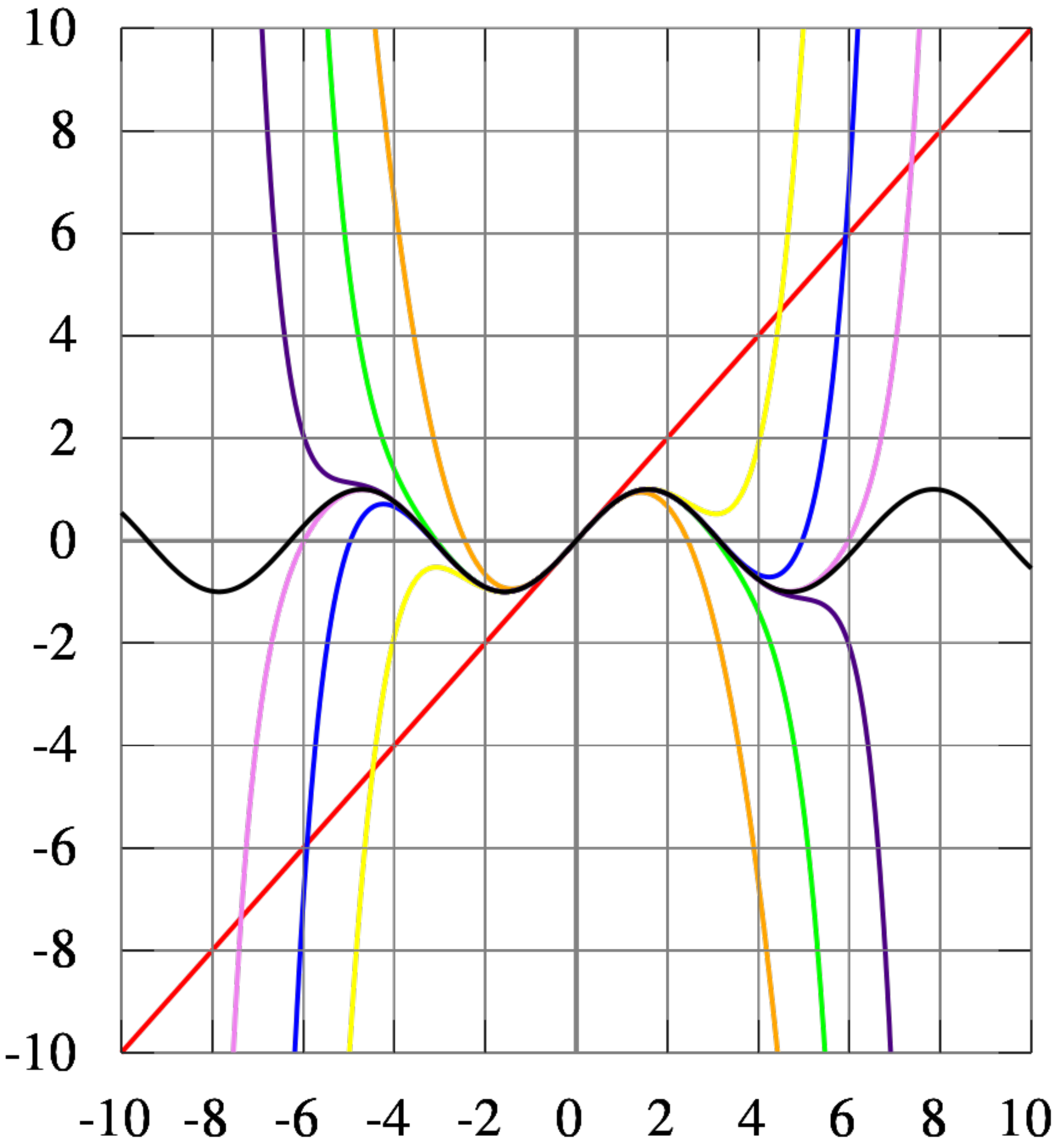


Taylor Series Visualization (2)

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

Approximating sin function
at point x0 = 0
(How can you tell?)

degree 1, 3, 5, 7, 9, 11 and 13.



Taylor Series

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$$= c(a) + \sum_{i=1}^{k} \frac{c^{(i)}(a)}{i!}(w-a)^i$$

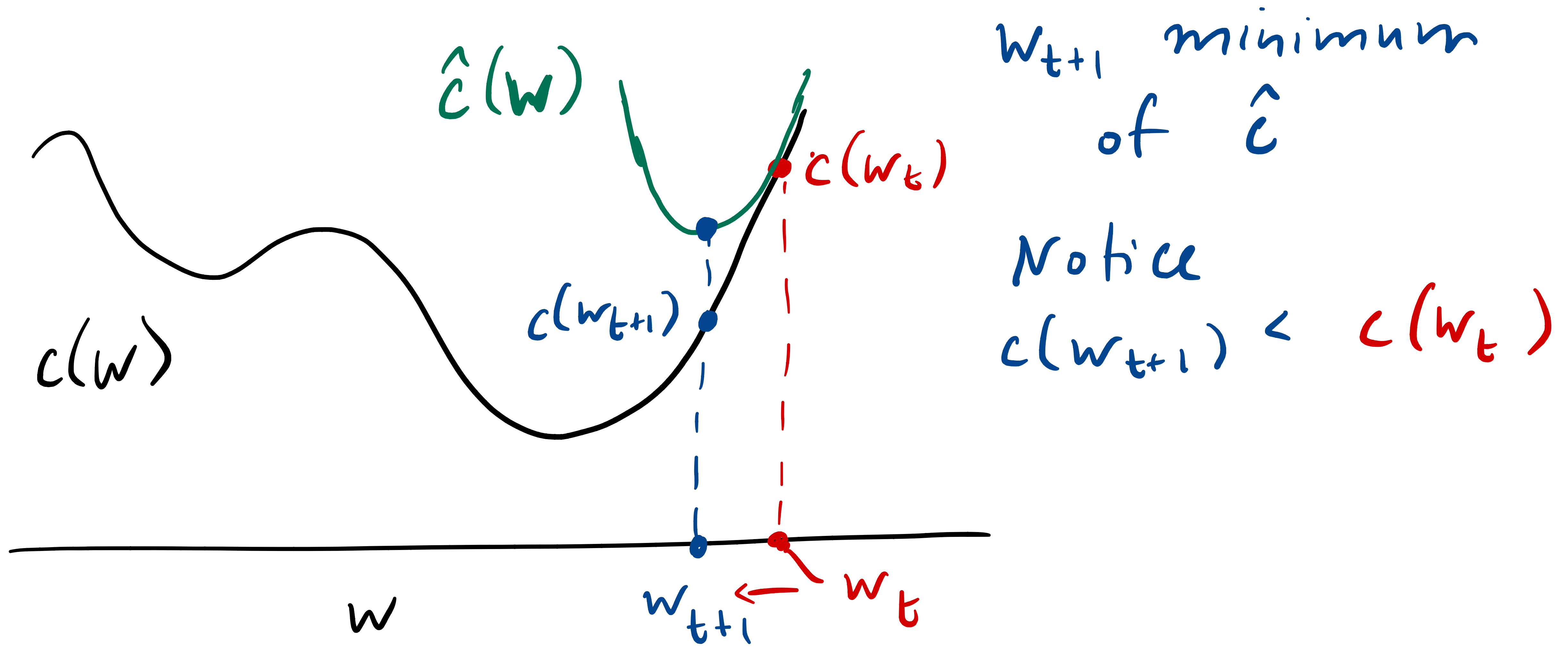
- *Intuition:* Following tangent line of the function approximates how it changes
  - i.e., following a function with the same first derivative
  - Following a function with the same first and second derivatives is a better approximation; with the same first, second, third derivatives is even better; etc.

Second-Order Gradient Descent (Newton-Raphson Method)

1. Approximate the target function with a **second-order Taylor series** around the current guess w_t: $$\hat{c}(w) = c(w_t) + c'(w_t)(w - w_t) + \frac{c''(w_t)}{2}(w - w_t)^2$$

2. Find the stationary point of the approximation

$$w_{t+1} \leftarrow w_t - \frac{c'(w_t)}{c''(w_t)}$$



Second-Order Gradient Descent

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2. Find the stationary point of the approximation

$$w_{t+1} \leftarrow w_t - \frac{c'(w_t)}{c''(w_t)}$$

3. If the stationary point of the approximation is a (good enough) stationary point of the objective, then stop. Else, goto 1.

$$0 = \frac{d}{dw}\left[c(a) + c'(a)(w - a) + \frac{c''(a)}{2}(w - a)^2\right]$$

$$= c'(a) + 2\frac{c''(a)}{2}w - 2\frac{c''(a)}{2}a$$

$$= c'(a) + c''(a)(w - a)$$

$$\iff -c'(a) = c''(a)(w - a)$$

$$\iff (w - a) = -\frac{c'(a)}{c''(a)}$$

$$\iff w = a - \frac{c'(a)}{c''(a)}$$

(First-Order) Gradient Descent

- We can run Second-order GD whenever we have access to both the first and second derivatives of the target function
- Often we want to only use the **first derivative**
  - Not obvious yet why, but for the multivariate case second-order is computationally intensive
- **First-order gradient descent:** Replace the **second derivative** with a constant $\frac{1}{\eta}$ (the **step size**) in the approximation:

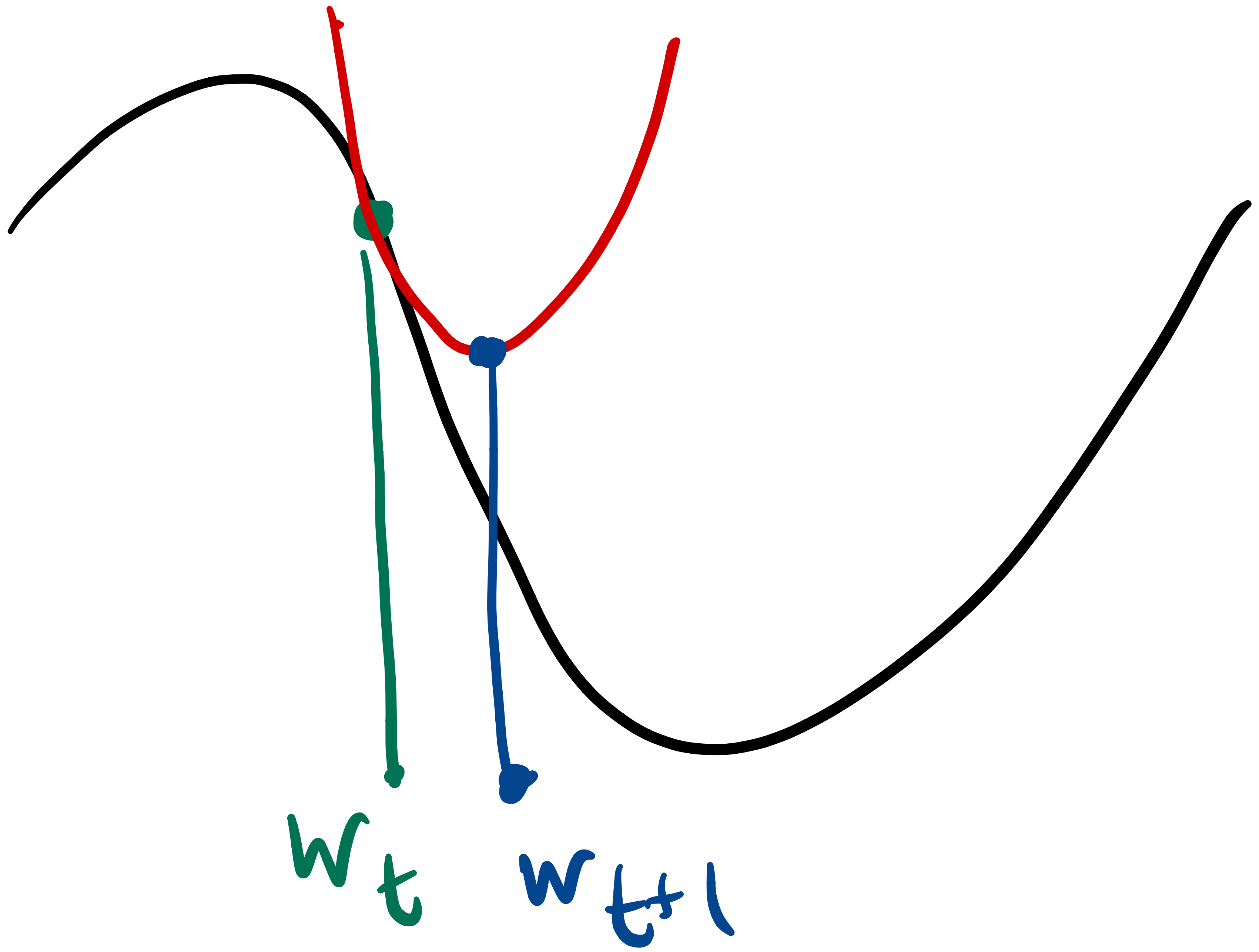
$$\hat{c}(w) = c(w_t) + c'(w_t)(w - w_t) + \frac{c''(w_t)}{2}(w - w_t)^2$$

$$\hat{c}(w) = c(w_t) + c'(w_t)(w - w_t) + \frac{1}{2\eta}(w - w_t)^2$$

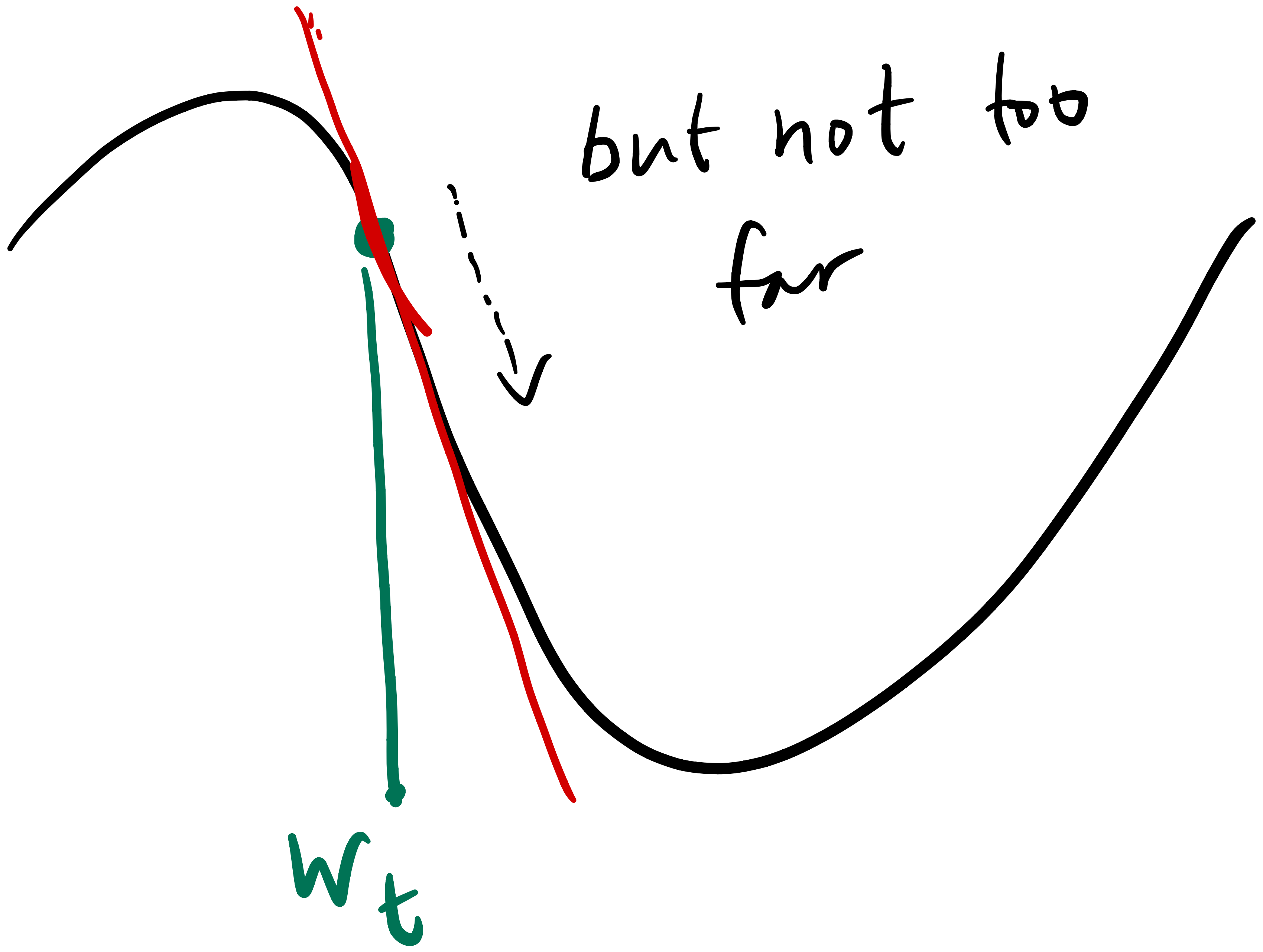
- By exactly the same derivation as before:

$$w_{t+1} \leftarrow w_t - \eta c'(w_t)$$

1st and 2nd order



2nd order



1st order, distance controlled by stepsize

Partial Derivatives

- **So far:** Optimizing univariate function $c : \mathbb{R} \to \mathbb{R}$
- **But actually:** Optimizing multivariate function $c : \mathbb{R}^d \to \mathbb{R}$
  - d is typically **H U G E** ($d \gg 10{,}000$ is not uncommon)
- First derivative of a multivariate function is a vector of partial derivatives

Definition:

The **partial derivative** $\dfrac{\partial f}{\partial x_i}(x_1, \ldots, x_d)$

of a function $f(x_1, \ldots, x_d)$ at $x_1, \ldots, x_d$ with respect to x_i **is** $g'(x_i)$, where

$$g(y) = f(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_d)$$

Example

- $c(w_1, w_2) = (2w_1 + 4w_2 - 7)^2$
- $\dfrac{\partial c}{\partial w_1}(w_1, w_2) = 4(2w_1 + 4w_2 - 7)$
- Then we query at a particular point, e.g., $(w_1, w_2) = (1, -1)$, giving $\dfrac{\partial c}{\partial w_1}(1, -1) = 4(2 - 4 - 7) = -36$
- Equivalently, let $f(w_1) = c(w_1, -1)$ for this fixed w_2
- Then $f'(w_1) = \dfrac{\partial c}{\partial w_1}(w_1, -1)$, i.e., $f'(1) = \dfrac{\partial c}{\partial w_1}(1, -1) = -36$

Gradients

The multivariate analog to a **first derivative** is called a **gradient**.

Definition:

The **gradient** $\nabla f(\mathbf{x})$ of a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ at $\mathbf{x} \in \mathbb{R}^d$ is a vector of all the partial derivatives of f at $\mathbf{x}$:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial_{x_1}}(\mathbf{x}) \\ \frac{\partial f}{\partial_{x_2}}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial_{x_d}}(\mathbf{x}) \end{bmatrix}$$

Multivariate Gradient Descent

First-order gradient descent for multivariate functions $c : \mathbb{R}^d \rightarrow \mathbb{R}$ is just:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta \nabla c(\mathbf{w}_t)$$

$$\begin{bmatrix} w_{t+1,1} \\ w_{t+1,2} \\ \vdots \\ w_{t+1,d} \end{bmatrix} = \begin{bmatrix} w_{t,1} \\ w_{t,2} \\ \vdots \\ w_{t,d} \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial c}{\partial_{w_1}}(\mathbf{w}_t) \\ \frac{\partial c}{\partial_{w_2}}(\mathbf{w}_t) \\ \vdots \\ \frac{\partial c}{\partial_{w_d}}(\mathbf{w}_t) \end{bmatrix}$$

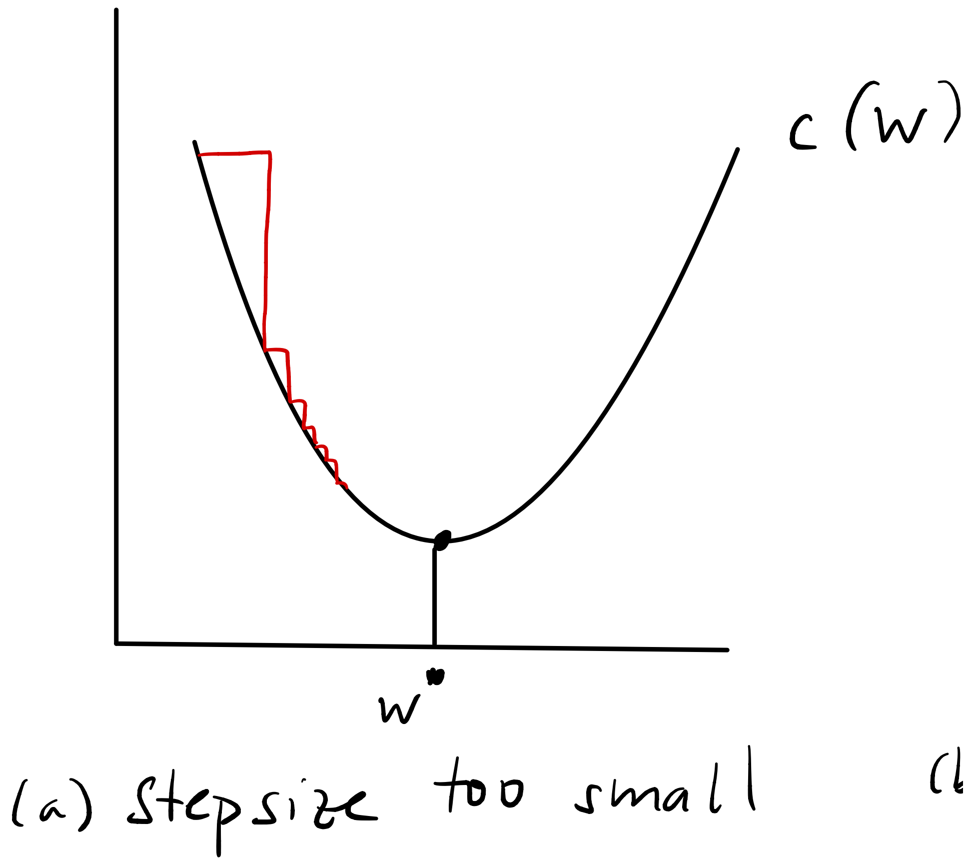
Extending to stepsize per timestep

First-order gradient descent for multivariate functions $c : \mathbb{R}^d \to \mathbb{R}$ is just:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla c(\mathbf{w}_t)$$

- Notice the t subscript on η
- We can choose a **different** η_t for each iteration
  - Indeed, for univariate functions, Newton-Raphson can be understood as first-order gradient descent that chooses a step size of $\eta_t = \dfrac{1}{c''(w_t)}$ at each iteration.
- Choosing a good step size is crucial to efficiently using first-order gradient descent

Adaptive Step Sizes



- If the step size is **too small**, gradient descent will "work", but take forever
- **Too big**, and we can overshoot the optimum
- There are some heuristics that we can use to **adaptively** guess good values for η_t
- Ideally, we would choose $\eta_t = \arg\min_{\eta \in \mathbb{R}^+} c\left(\mathbf{w}_t - \eta \nabla c(\mathbf{w}_t)\right)$
  - But that's another optimization!

Line Search

A simple heuristic: **line search**

1. Try some largest-reasonable step size $\eta_t^{(0)} = \eta_{\text{max}}$
2. Is $c\left(w_t - \eta_t^{(s)} \nabla c(w_t)\right) < c(w_t)$?
   If yes, $w_{t+1} \leftarrow w_t - \eta_t^{(s)} \nabla c(w_t)$
3. Otherwise, try $\eta_t^{(s+1)} = \tau \eta_t^{(s)}$
   (for $\tau < 1$) and goto 2

Intuition:

- Big step sizes are better so long as they don't overshoot
- Try a big step size! If it *increases* the objective, we must have overshot, so try a smaller one.
- Keep trying smaller ones until you *decrease* the objective; then start iteration $t + 1$ from η_{max} again.

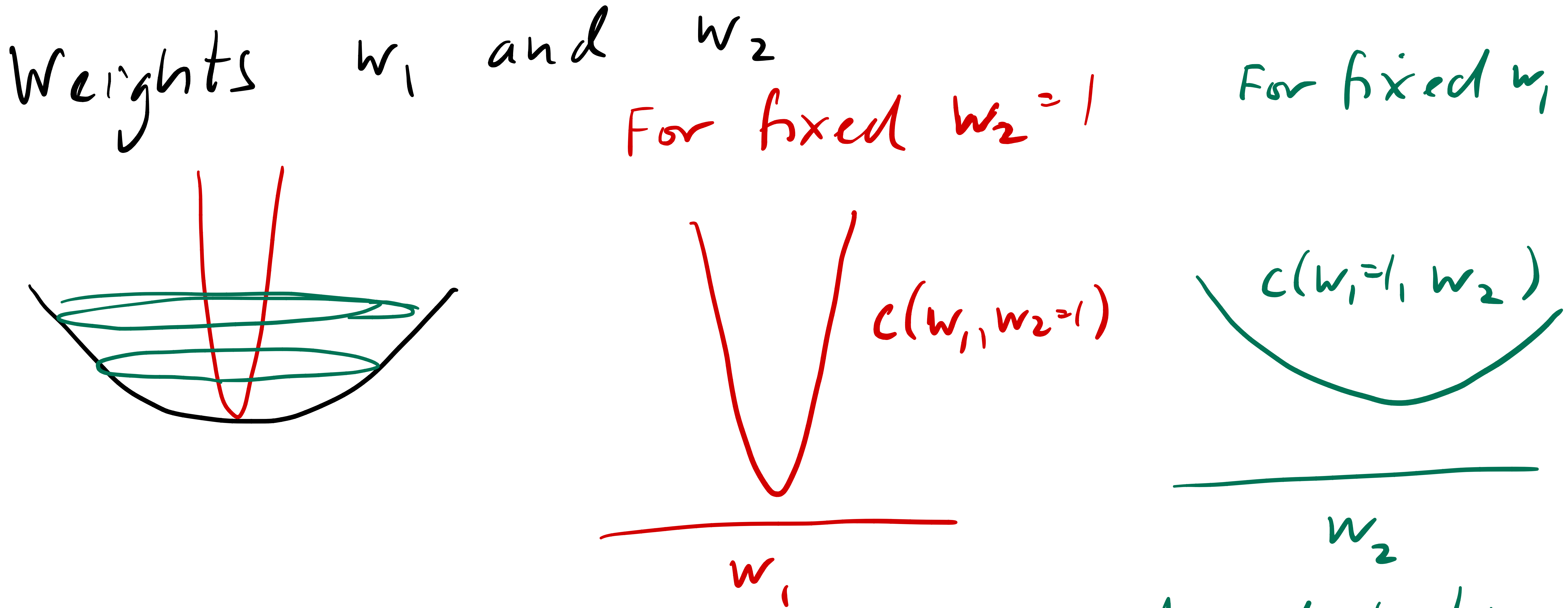
- Typically $\tau \in [0.5, 0.9]$

Adaptive stepsize algorithms

- Stepsize selection is very important, and so there is a vast array of algorithms for adaptive stepsizes
- Line search is a bit onerous to use, and not common with something called stochastic gradient descent (which is what we will use later)
- We will see smarter stepsize algorithms then, and in your assignment

Do we have to use a scalar stepsize?

- Or can we use a different stepsize per dimension? And why would we?



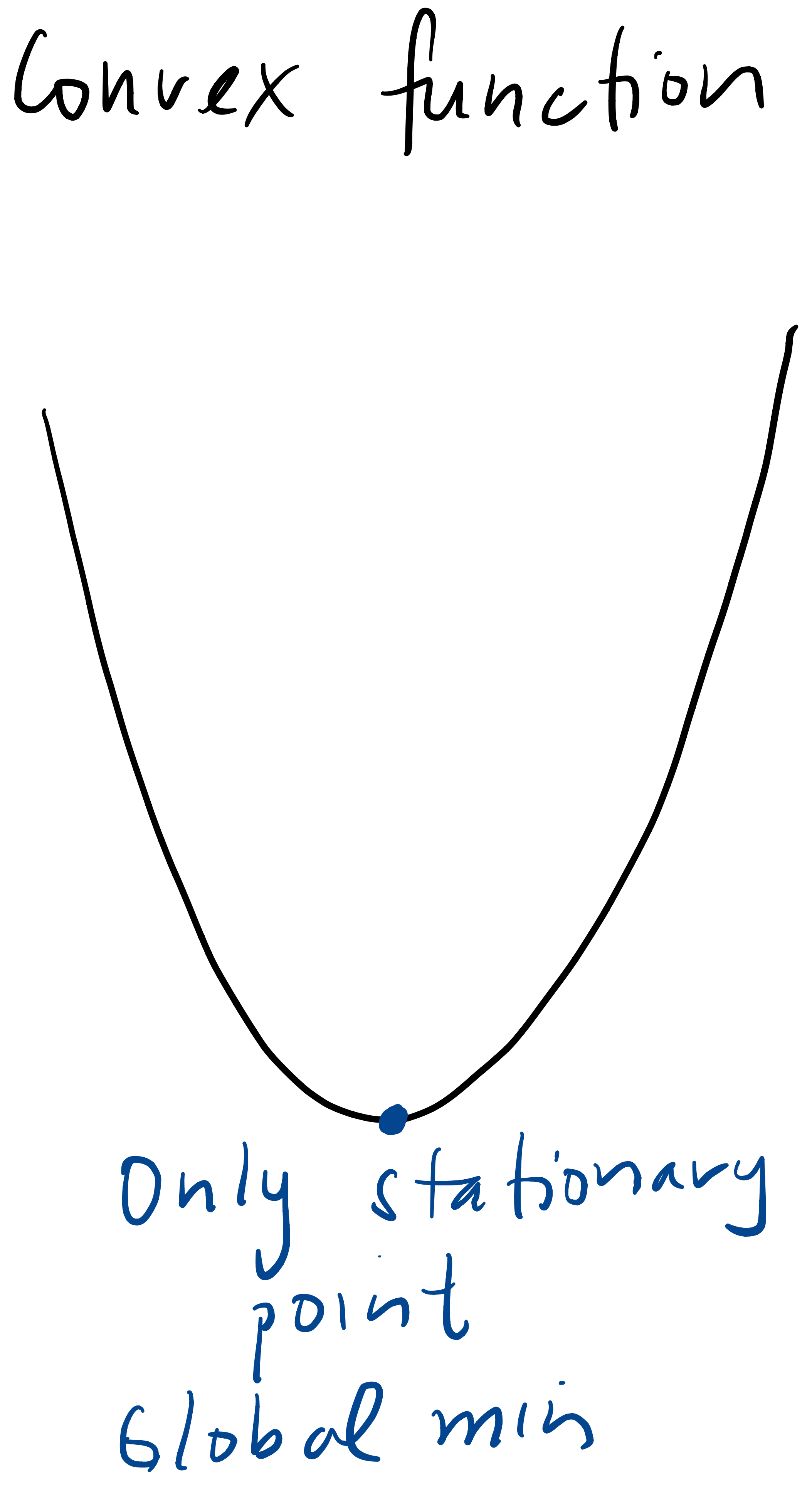
Stepsize 1 should be small

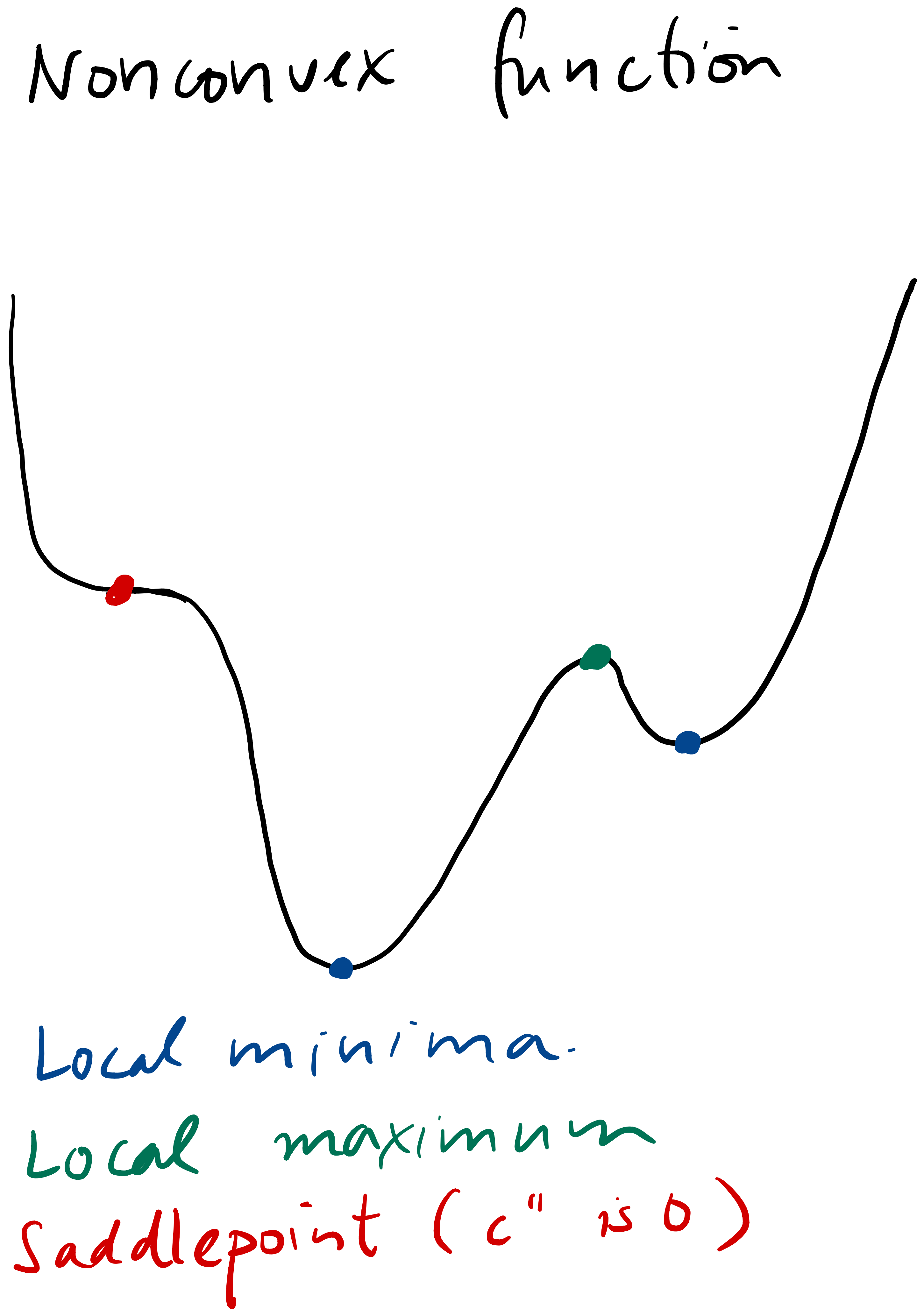
Stepsize 2 should be big

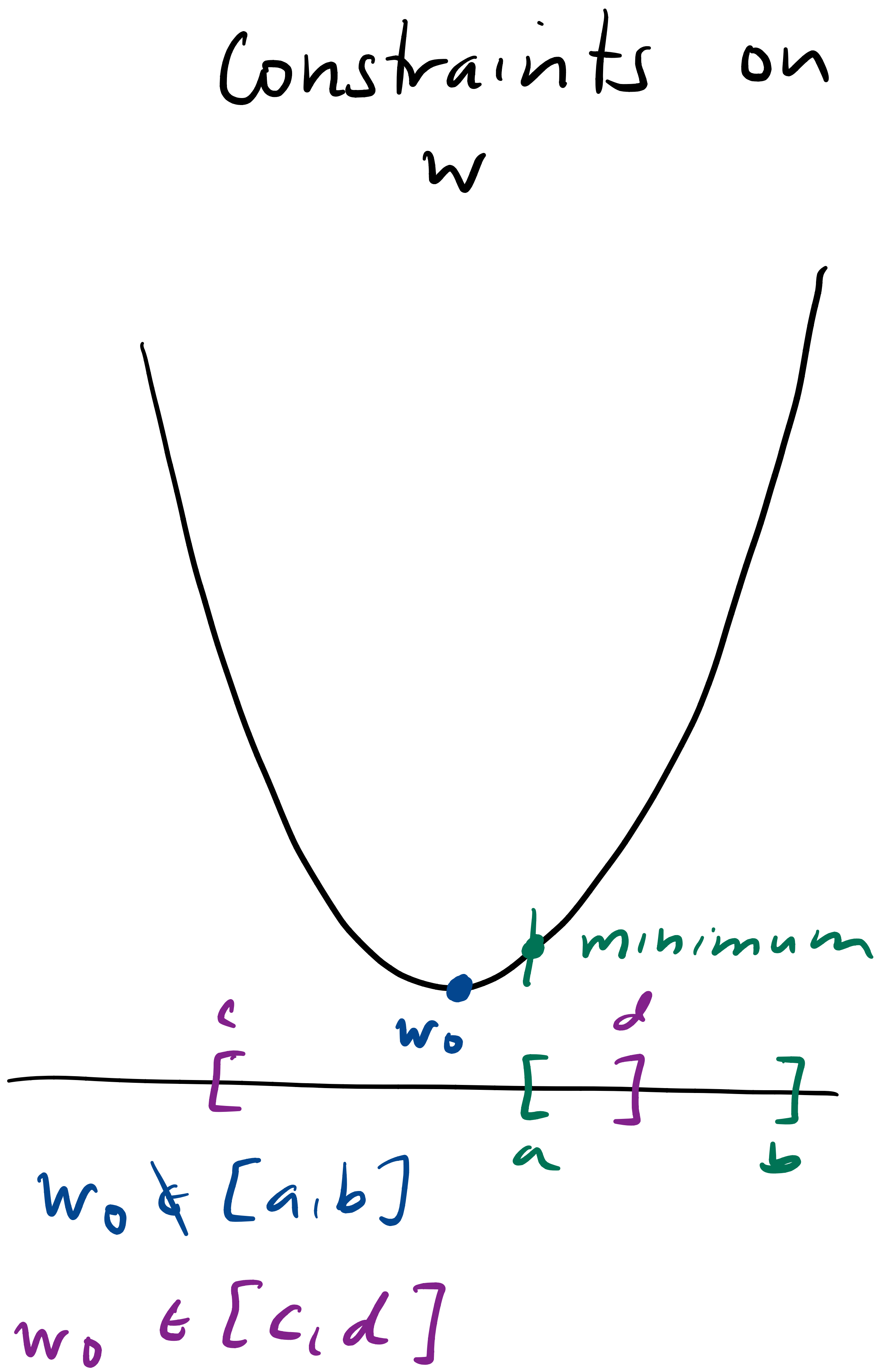
Now what if we have constraints?

- For this course, we almost always only deal with unconstrained problems
- We will only consider constraints like $w \geq 0$ or $w \in [a, b]$
- Then the procedure is:
  - 1. Find a stationary point
  - 2. Verify that it is the only stationary point, and a local min according to the second derivative test
  - 3. Additionally check if the boundary points have a smaller value

Visualizing the effect of constraints







Summary

- We often want to find the argument w^* that **minimizes** an **objective function** c:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} c(\mathbf{w})$$

- Every interior minimum is a **stationary point**, so check the stationary points
- Stationary points usually identified **numerically**
  - Typically, by **gradient descent**
- Choosing the **step size** is important for efficiency and correctness
  - Common approach: Adaptive step size
  - E.g., by **line search**