10-301/601: Introduction to Machine Learning
Lecture 8 – Optimization for Machine Learning

Geoff Gordon

with thanks to Henry Chai & Matt Gormley

HW3 out

- Check the Coursework tab and our HW3 FAQ post
- Due Monday Sep 27 11:59pm (CMU time)
- Written only (no programming)
- Only 2 grace days allowed (later would go too close to the exam)

Quiz 1 logistics

- Right here, during usual class period on Friday
- First 20 minutes, followed by regular recitation
- Everyone has an assigned seat for the quiz—see Piazza
  - check **today** to make sure you know your seat
  - if you're not on the seating chart, it means we think **you** have made arrangements with ODR for them to proctor—if that's not true, contact us ASAP!
- Questions: reading and writing short Python programs related to HW1 and HW2
  - no, small syntax errors will not cause you to get the whole question wrong

Exam 1 logistics

- Note evening time (not during regular class slot)
  - 7pm Mon Sep 29
- Location & Seats: You will be split across multiple (large) rooms, and everyone will have an assigned seat (chart to be posted on Piazza)
- One letter-sized sheet of notes (both sides); no devices
- If you have exam accommodations through ODR, they will be proctoring your exam on our behalf (and you won’t be in the seating chart); **you must submit the proctoring request through your student portal**

Exam 1 Topics

- Covered material: Lectures 1 – 7 (i.e., ***not today***)
  - Foundations
    - Probability, Linear Algebra, Geometry, Calculus
    - Optimization
  - Important Concepts
    - Overfitting
    - Model selection / Hyperparameter optimization
  - Decision Trees
  - k-NN
  - Perceptron
  - Regression
    - Decision Tree and k-NN Regression
    - Linear Regression

Exam 1 Preparation

- Attend the midterm review OH! (recitation slot this Fri)
- Review the exam practice problems (to be released soon)
- Review HWs 1–3
- Consider whether you have achieved the “learning objectives” in our slides for each lecture / section
- Write your one-page cheat sheet (back and front)

Exam 1 Tips

- Solve the easy problems first
- If a problem seems extremely complicated, you might be missing something
- If you make an assumption, write it down
- Don’t leave any answer blank unless out of time
  - If you look at a question and don’t know the answer:
    - just start trying things
    - consider multiple approaches
    - imagine arguing for some answer and see if you like it

Recall: Gradient Descent for Linear Regression

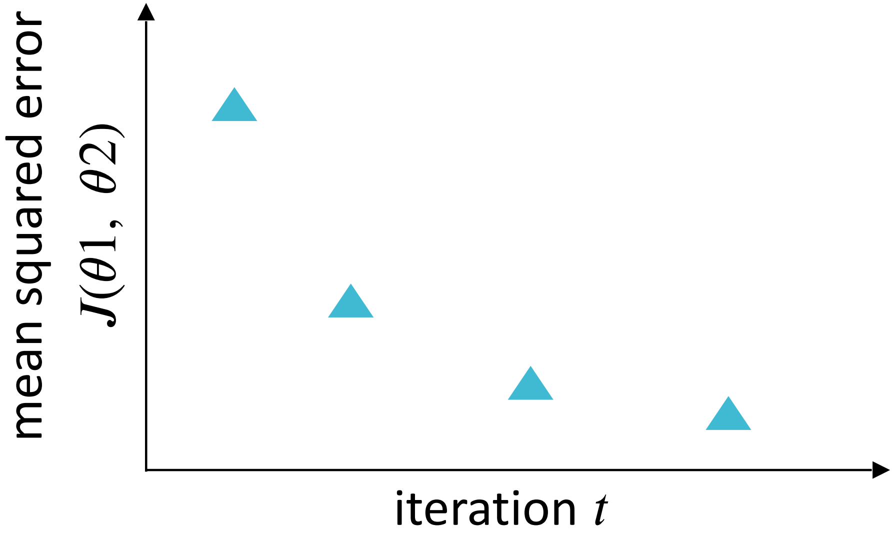
- Gradient descent for linear regression repeatedly takes steps opposite the gradient of the objective function

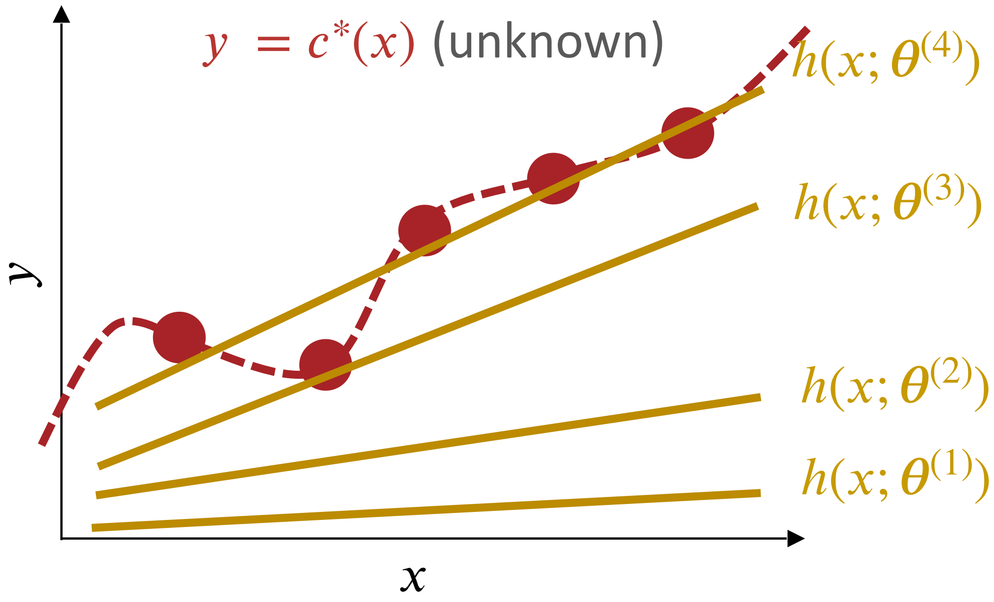
Algorithm 1 GD for Linear Regression

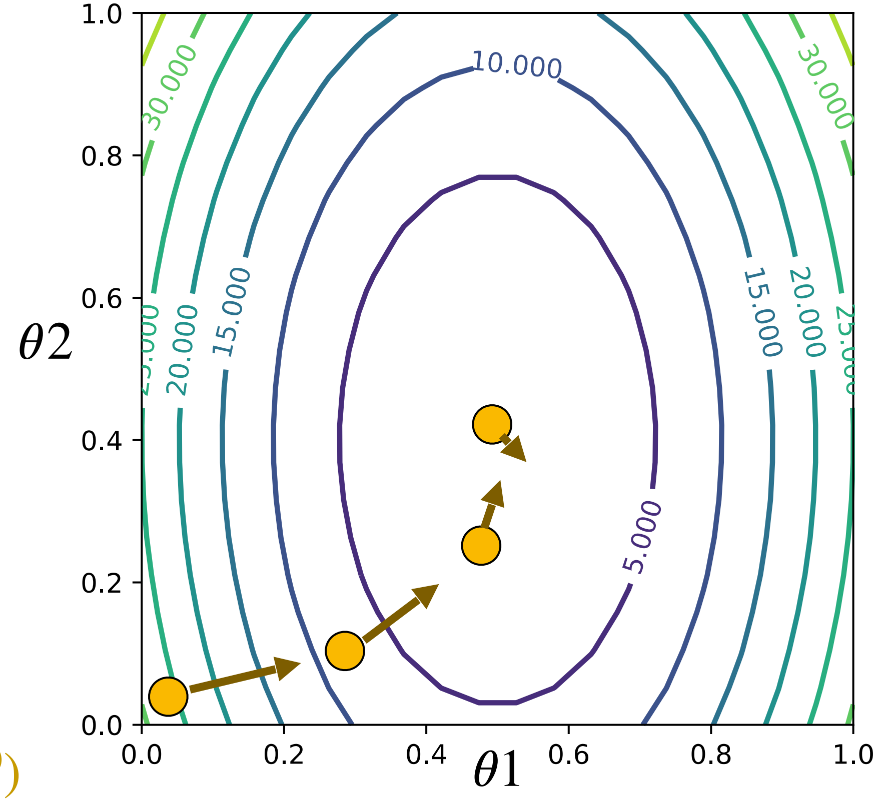
1: **procedure** GDLR($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
2: $\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ ▷ Initialize parameters
3: $\quad$**while** not converged **do**
4: $\quad\quad\mathbf{g} \leftarrow \sum_{i=1}^{N}(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})\mathbf{x}^{(i)}$ ▷ Compute gradient
5: $\quad\quad\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \mathbf{g}$ ▷ Update parameters
6: $\quad$**return** $\boldsymbol{\theta}$

Recall: Gradient Descent for Linear Regression

$$J(\theta_1,\ \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)}\right)^2$$







t	θ_1	θ_2	$J(\theta_1, \theta_2)$
1	0.01	0.02	25.2
2	0.30	0.12	8.7
3	0.51	0.30	1.5
4	0.59	0.43	0.2

Why Gradient Descent for Linear Regression?

- Globally convergent! (see below)
- Scalable: $O(MN)$ per iteration
  - "good enough" answer = not too many iterations
- Parallelizable: distribute gradient calculation across multiple GPUs or even a cluster
- Extensions (SGD, momentum, Adam, parameter server) are even more scalable (and sometimes parallelizable)
  - much faster per iteration, somewhat more iterations
- Works for a lot of models beyond just linear regression!

Convexity

- A function $f: \mathbb{R}^D \rightarrow \mathbb{R}$ is convex if

  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

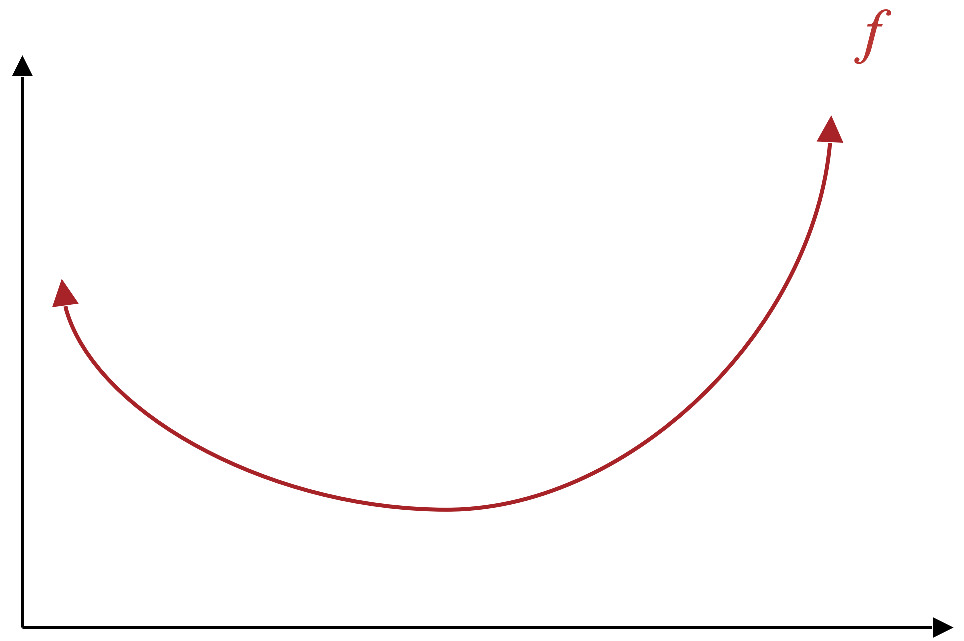
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq c f\left(\boldsymbol{x}^{(1)}\right) + (1-c) f\left(\boldsymbol{x}^{(2)}\right)$$

Convexity

- A function $f\colon \mathbb{R}^D \to \mathbb{R}$ is convex if

  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \le c \le 1$

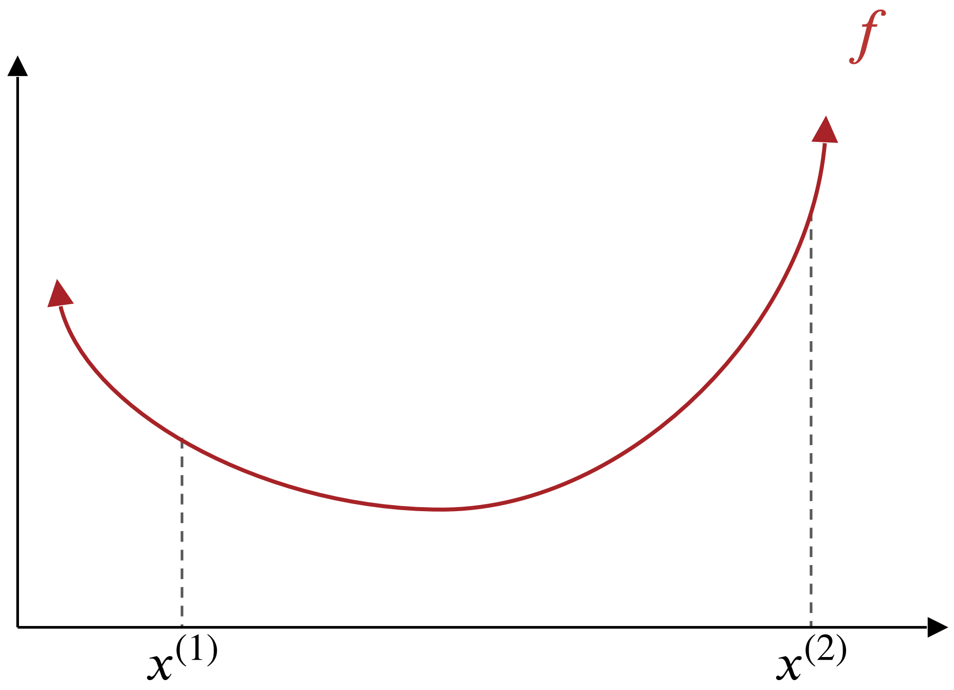
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \le c f\left(\boldsymbol{x}^{(1)}\right) + (1-c) f\left(\boldsymbol{x}^{(2)}\right)$$



Convexity

- A function $f\colon \mathbb{R}^D \to \mathbb{R}$ is convex if
  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \le c \le 1$

$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \le c f\left(\boldsymbol{x}^{(1)}\right) + (1-c) f\left(\boldsymbol{x}^{(2)}\right)$$

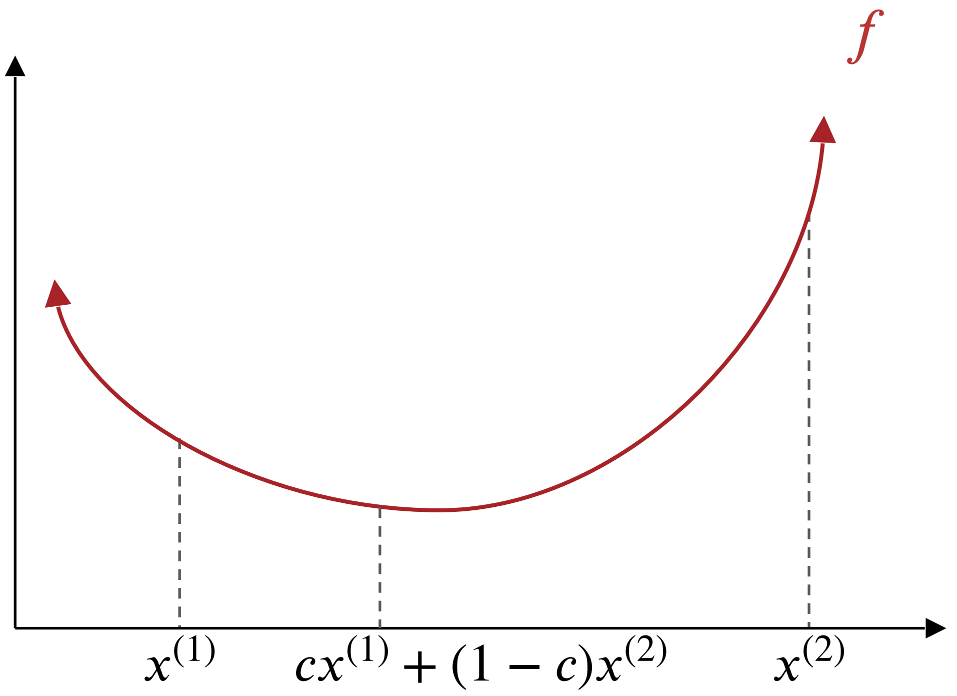


Convexity

- A function $f: \mathbb{R}^D \rightarrow \mathbb{R}$ is convex if

  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$

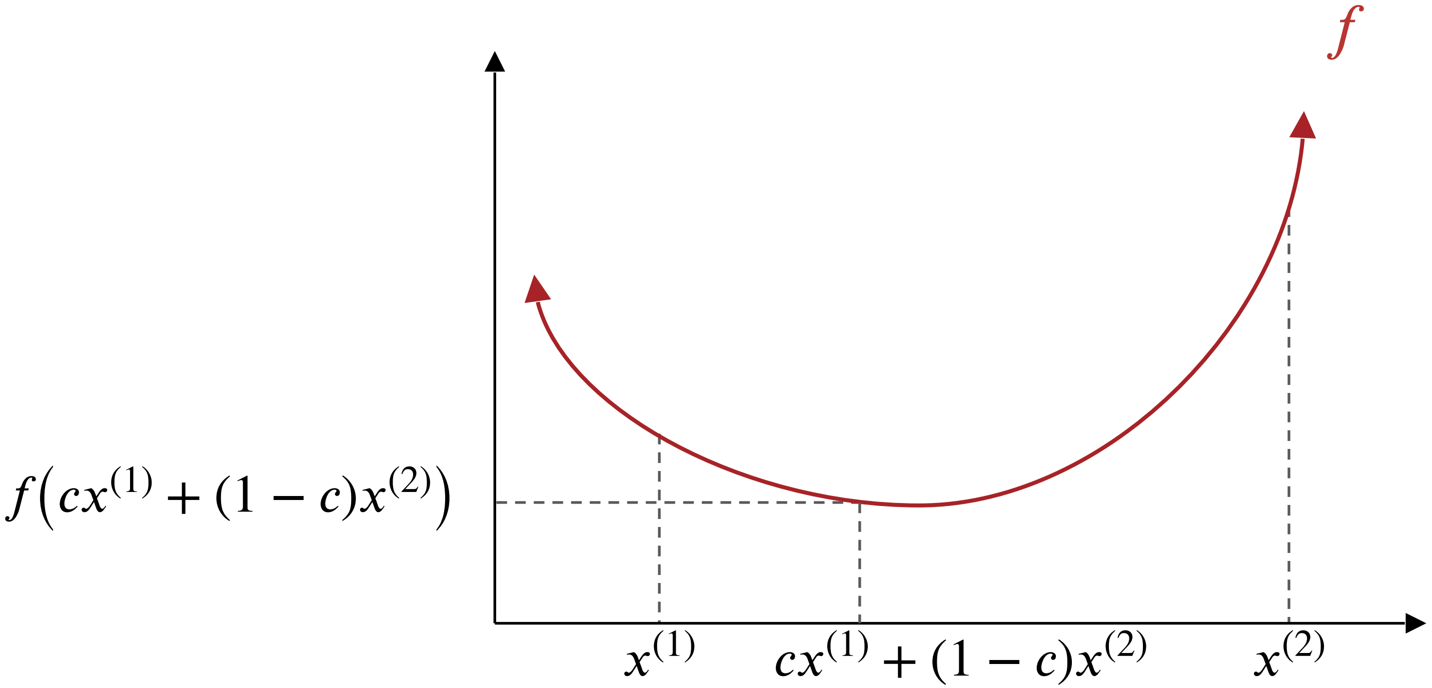


Convexity

- A function $f\colon \mathbb{R}^D \rightarrow \mathbb{R}$ is convex if

  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

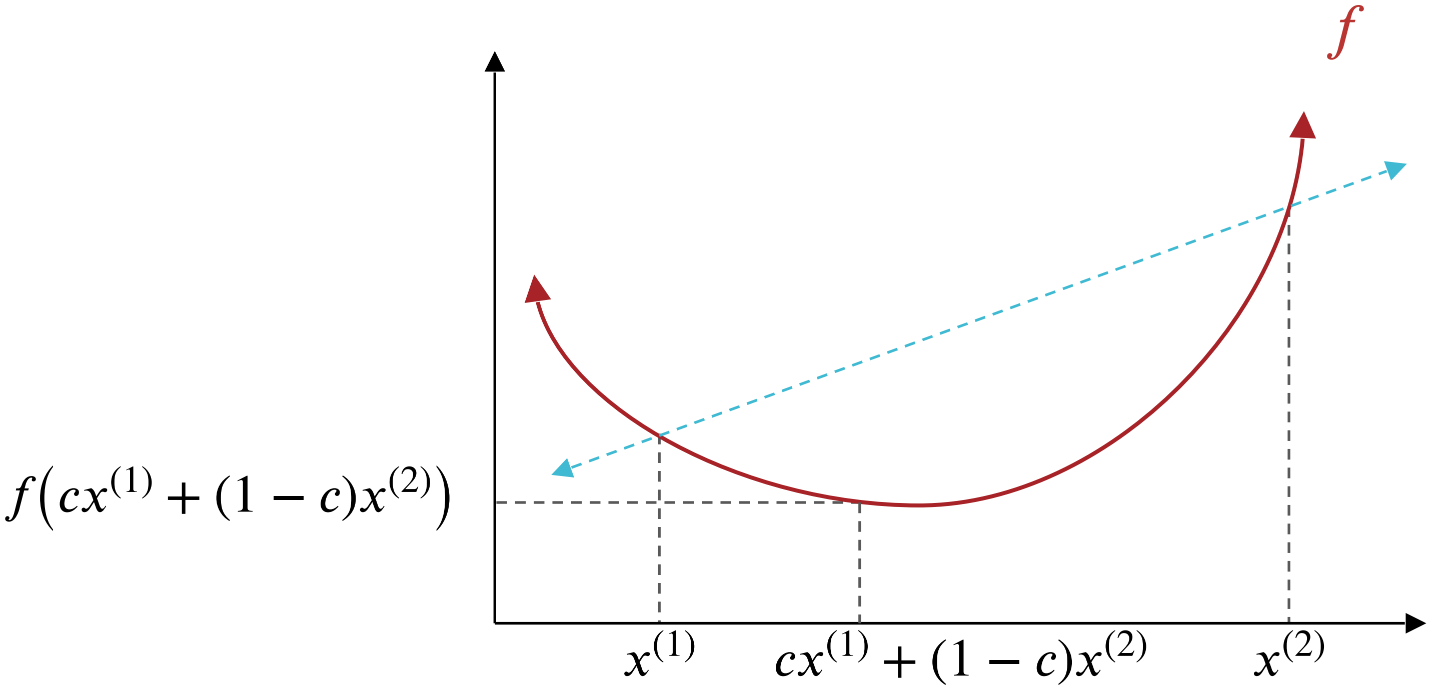
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq c f\left(\boldsymbol{x}^{(1)}\right) + (1-c) f\left(\boldsymbol{x}^{(2)}\right)$$



Convexity

- A function $f: \mathbb{R}^D \to \mathbb{R}$ is convex if
  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

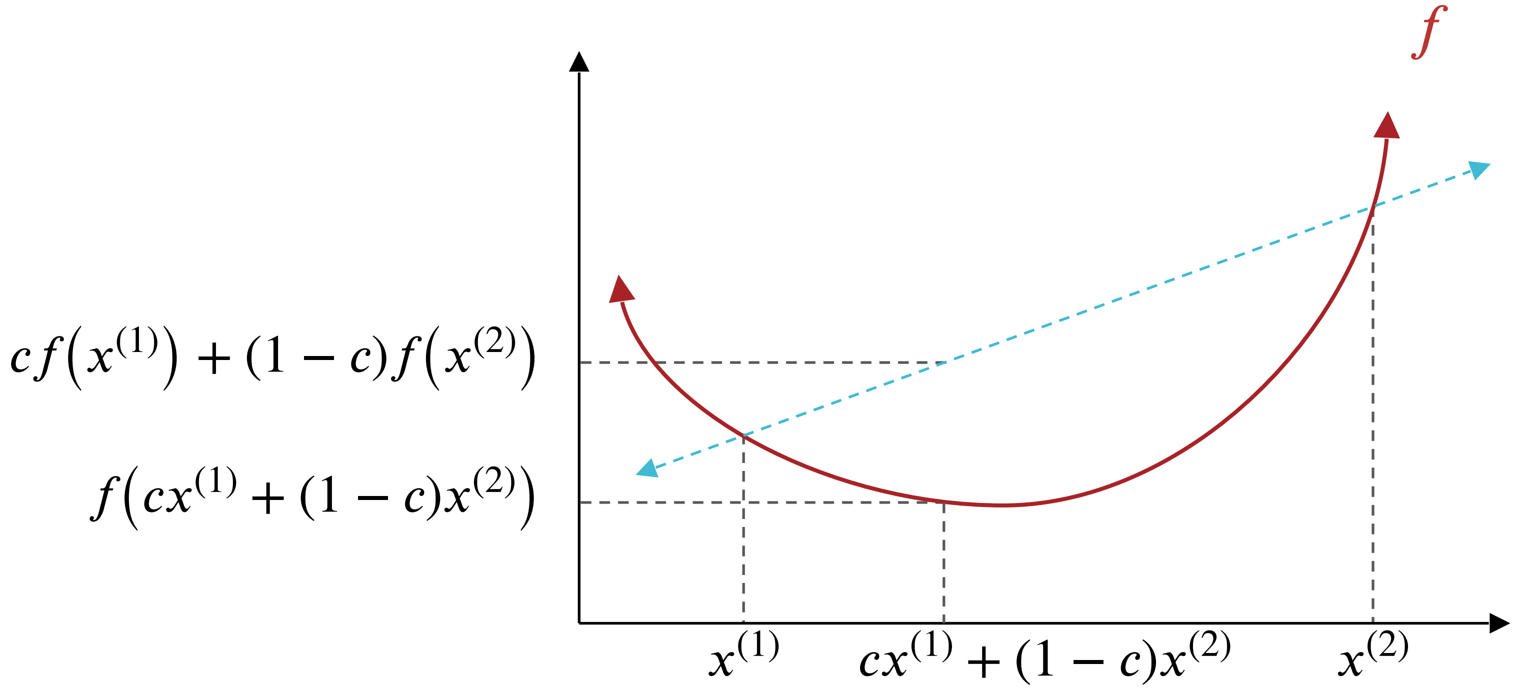
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



Convexity

- A function $f\colon \mathbb{R}^D \to \mathbb{R}$ is convex if $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

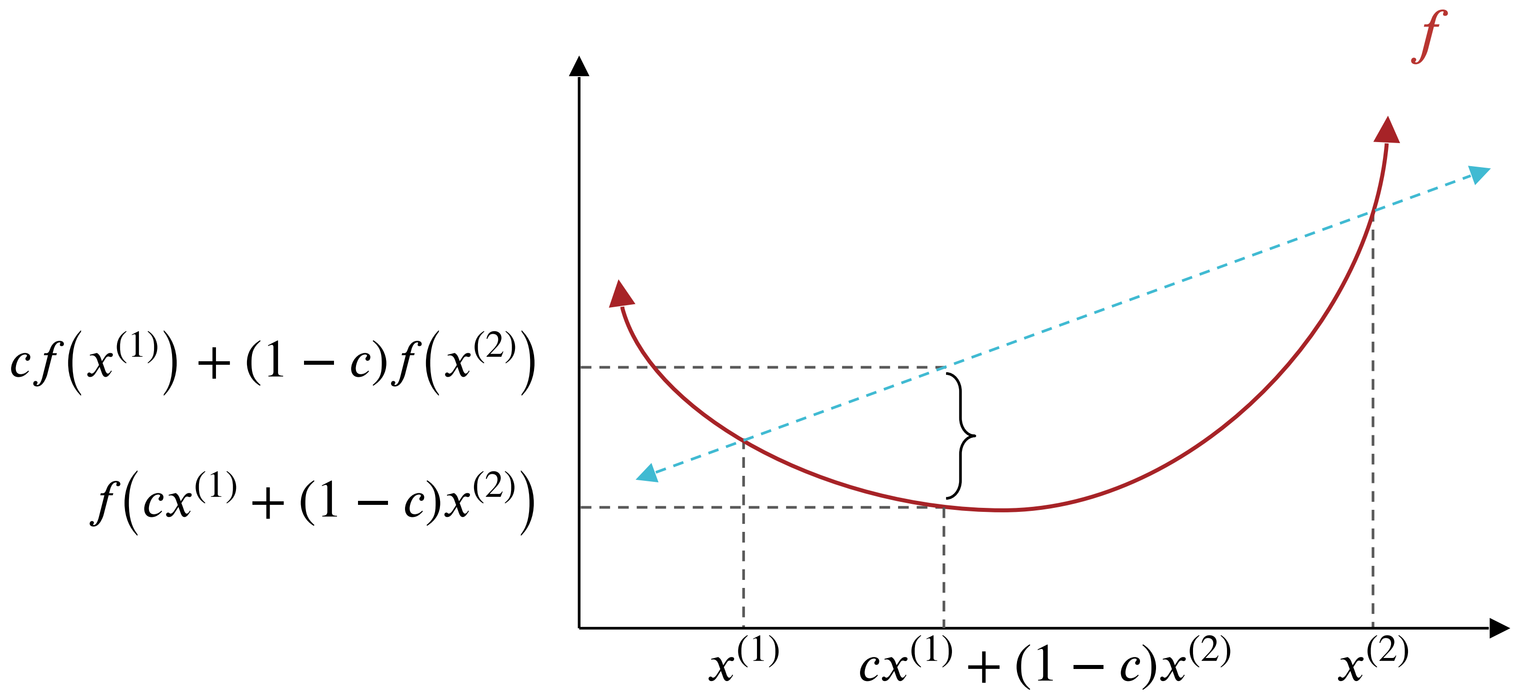
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq c f\left(\boldsymbol{x}^{(1)}\right) + (1-c) f\left(\boldsymbol{x}^{(2)}\right)$$



Convexity

- A function $f\colon \mathbb{R}^D \to \mathbb{R}$ is convex if
  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \leq c \leq 1$

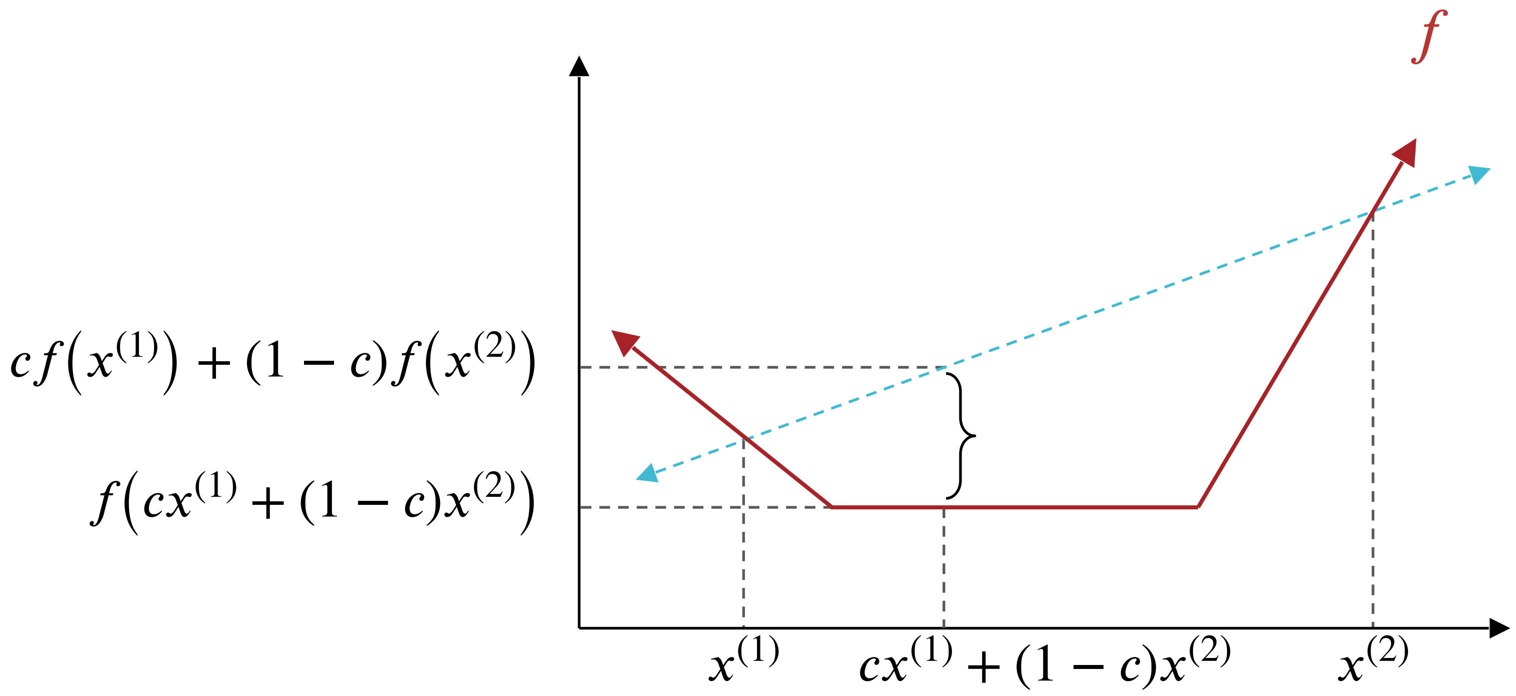
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \leq cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



Convexity

- A function $f\colon \mathbb{R}^D \to \mathbb{R}$ is convex if
  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 \le c \le 1$

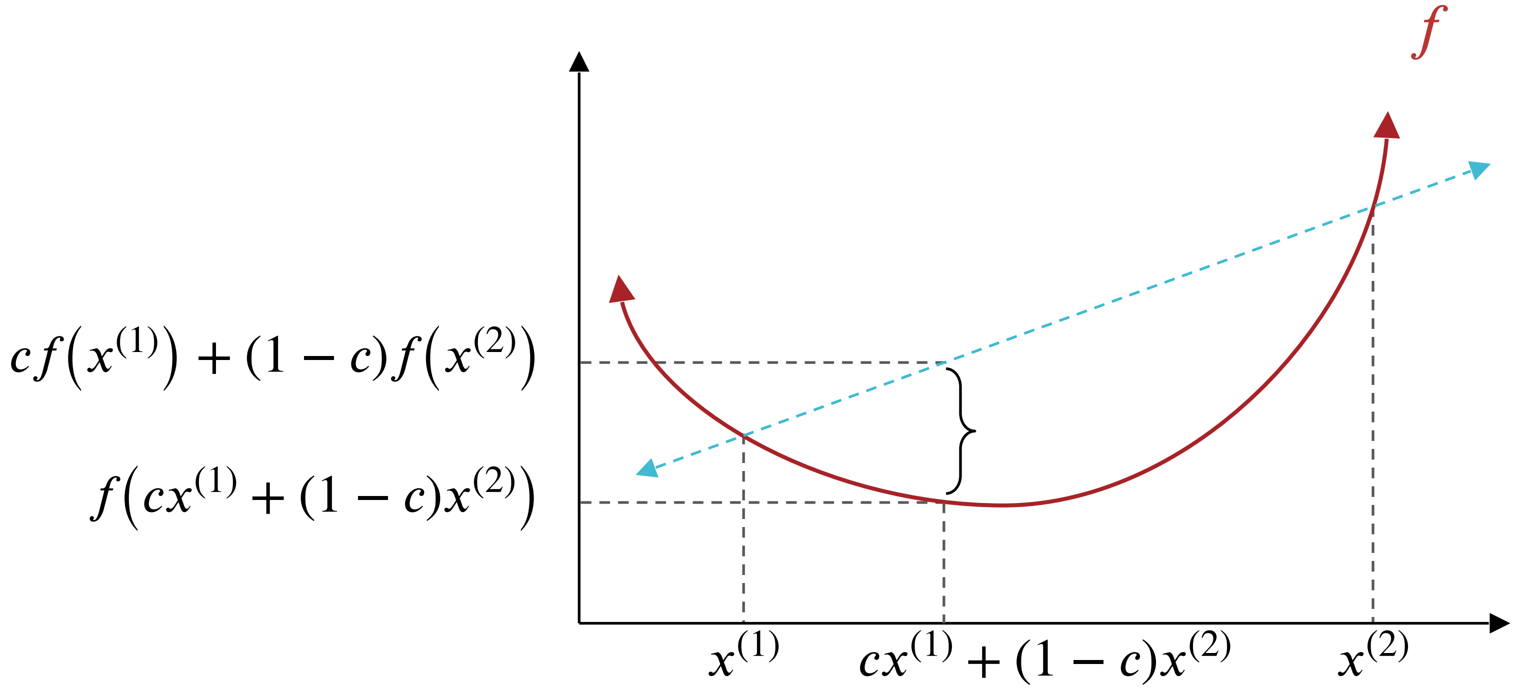
$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) \le cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$



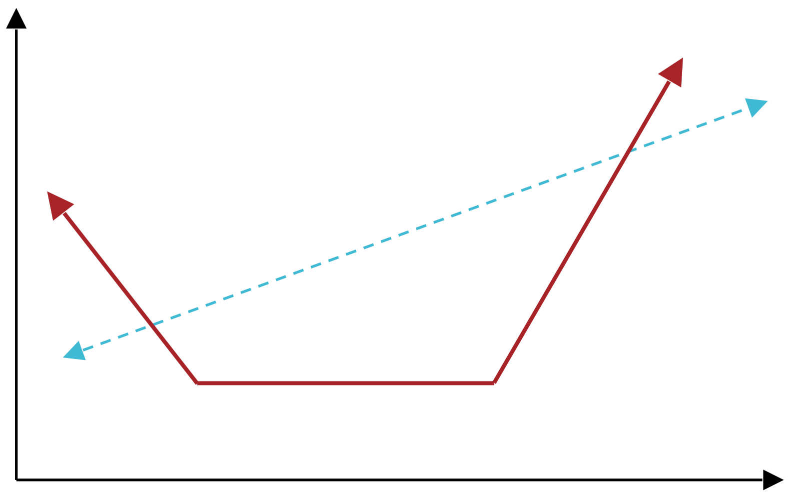
Convexity

- A function $f\colon \mathbb{R}^D \rightarrow \mathbb{R}$ is *strictly* convex if
  $\forall\ \boldsymbol{x}^{(1)} \in \mathbb{R}^D, \boldsymbol{x}^{(2)} \in \mathbb{R}^D$ and $0 < c < 1$

$$f\left(c\boldsymbol{x}^{(1)} + (1-c)\boldsymbol{x}^{(2)}\right) < cf\left(\boldsymbol{x}^{(1)}\right) + (1-c)f\left(\boldsymbol{x}^{(2)}\right)$$

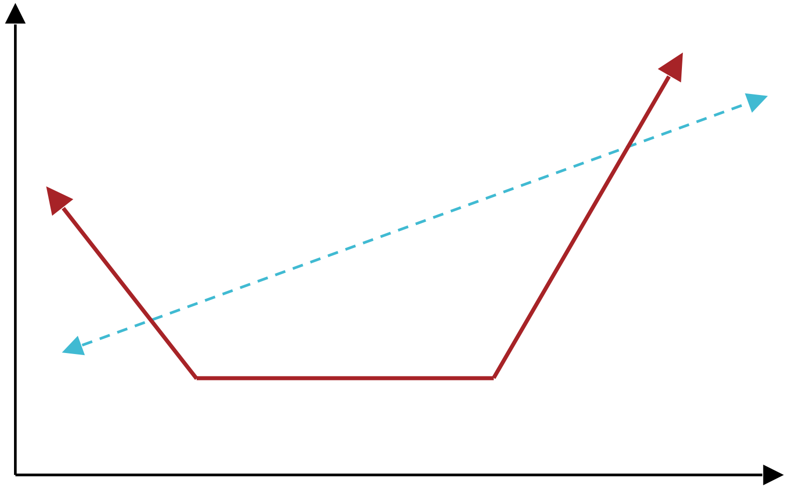


Convexity: local and global minima

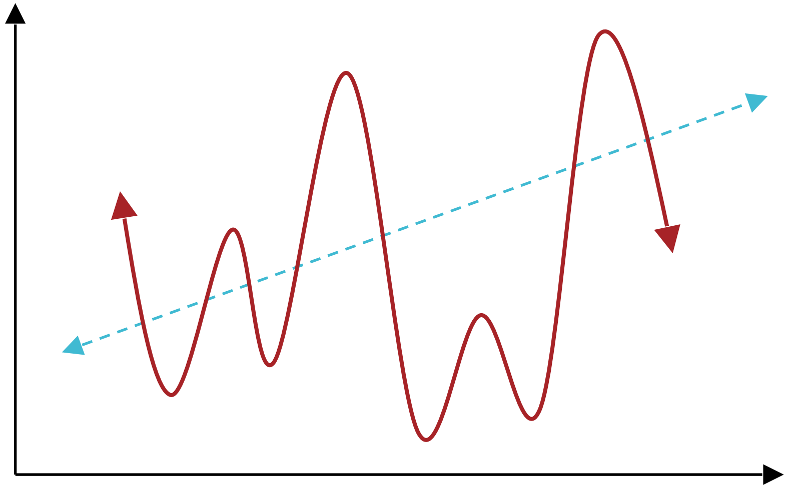


Convex functions

Convexity: local and global minima

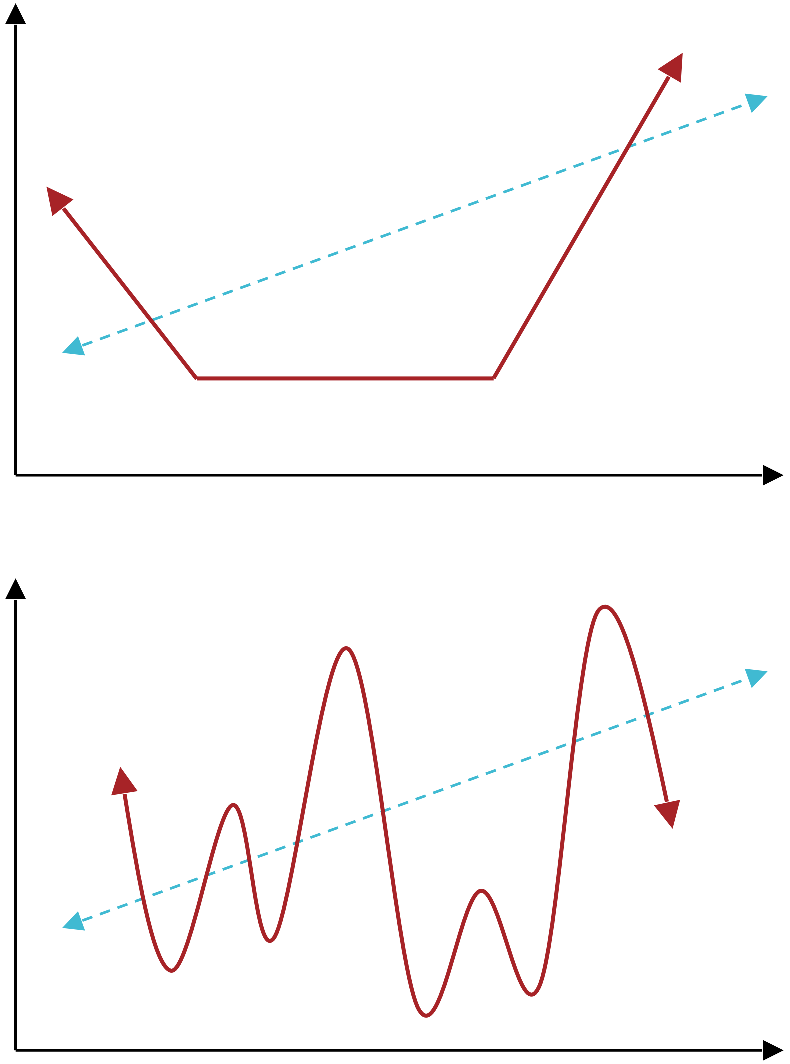


Convex functions



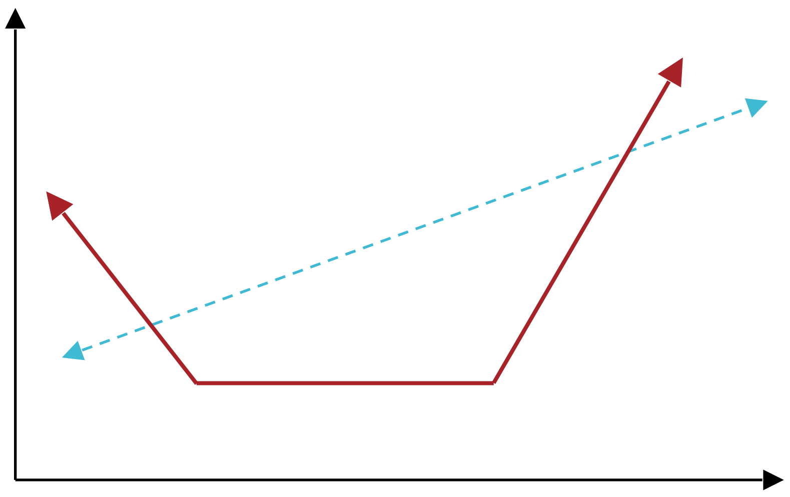
Non-convex functions

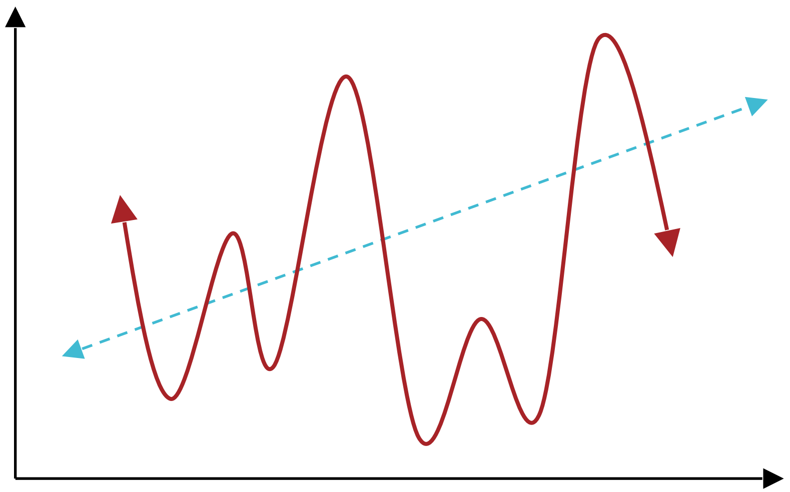
Convexity: local and global minima



Given a function $f\colon \mathbb{R}^D \to \mathbb{R}$

Convexity: local and global minima



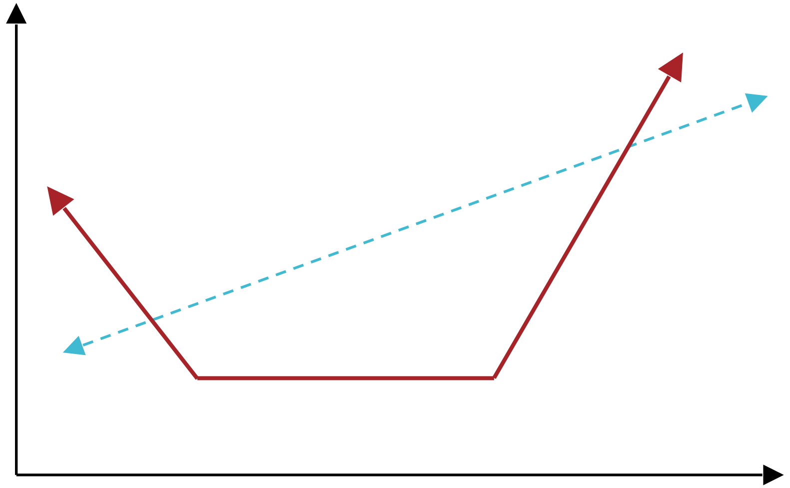


Given a function $f: \mathbb{R}^D \to \mathbb{R}$

- $\boldsymbol{x}^*$ is a global minimum iff

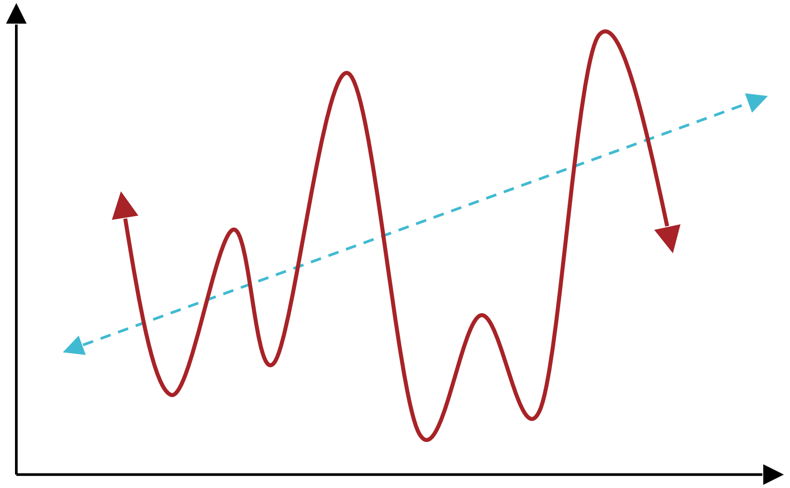
  $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \ \forall \ \boldsymbol{x} \in \mathbb{R}^D$

Convexity: local and global minima



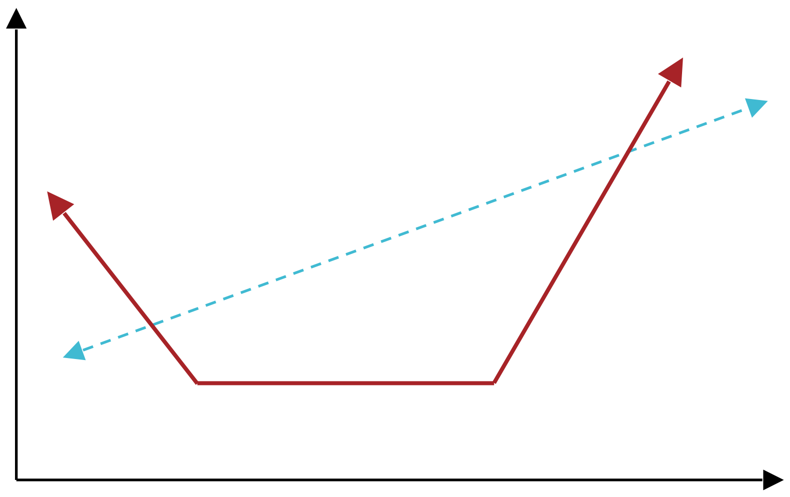
Given a function $f: \mathbb{R}^D \rightarrow \mathbb{R}$

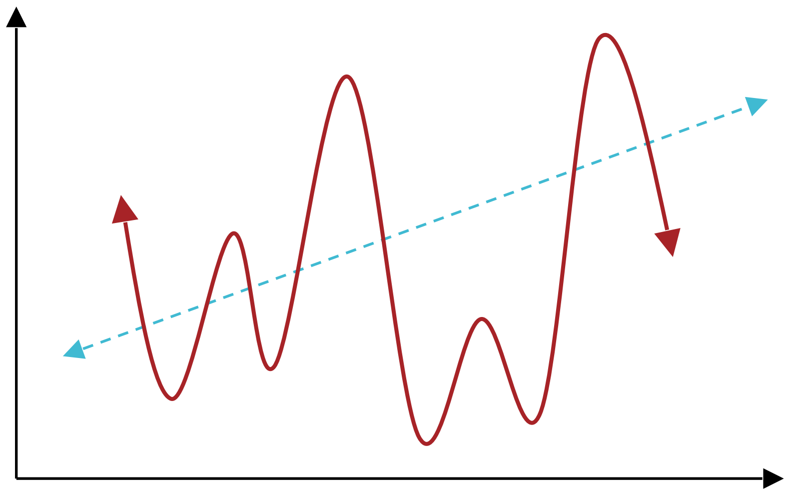
- $\boldsymbol{x}^*$ is a global minimum iff $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \; \forall \; \boldsymbol{x} \in \mathbb{R}^D$



- $\boldsymbol{x}^*$ is a local minimum iff $\exists \; \epsilon$ s.t. $f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \; \forall \; \boldsymbol{x} \text{ s.t. } \|\boldsymbol{x} - \boldsymbol{x}^*\|_2 < \epsilon$

Convexity: local and global minima

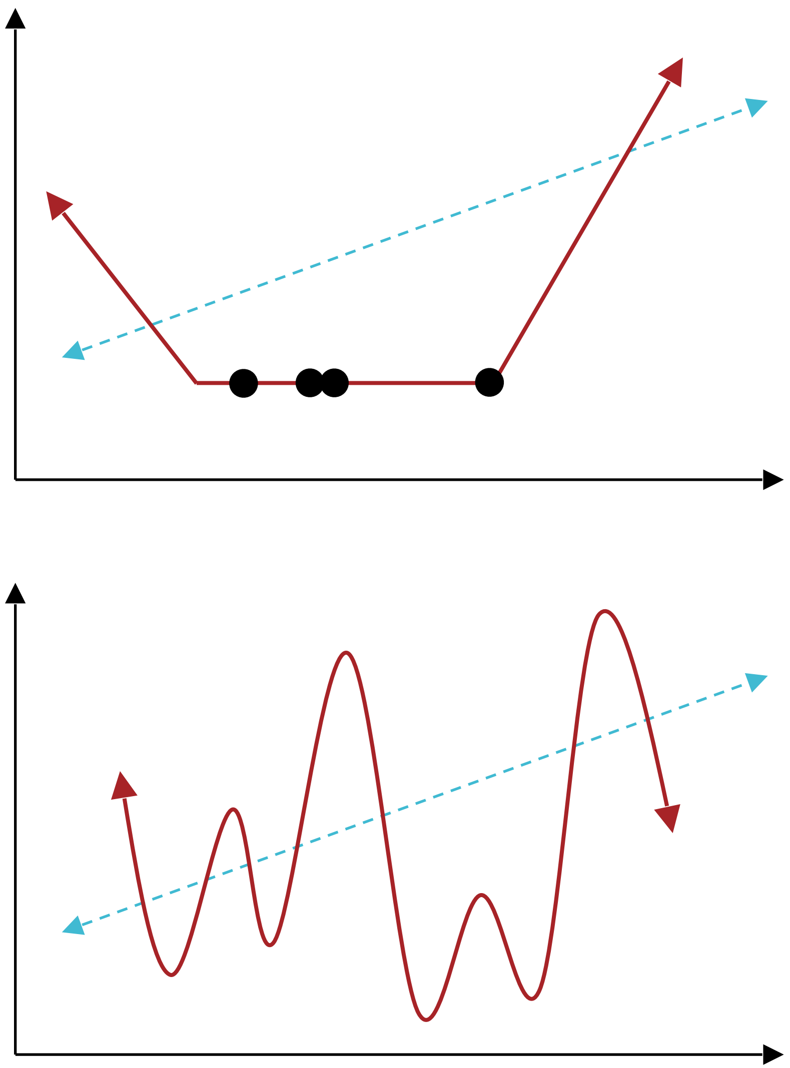




Convex functions:

Each local minimum is a global minimum!

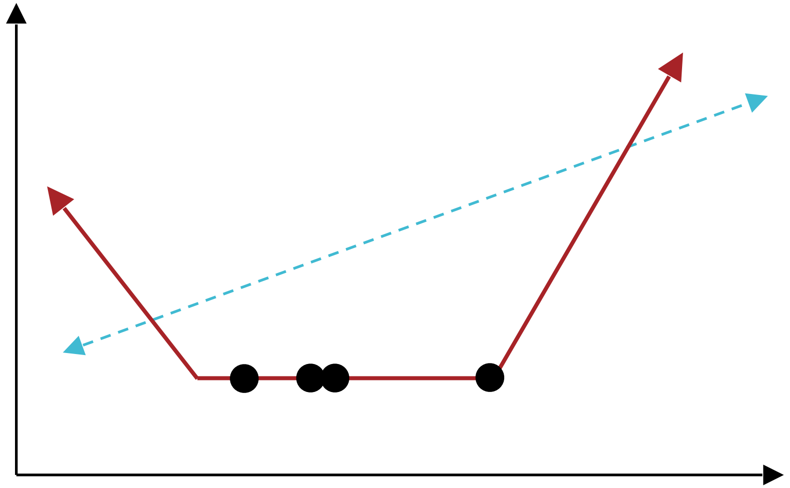
Convexity: local and global minima



Convex functions:

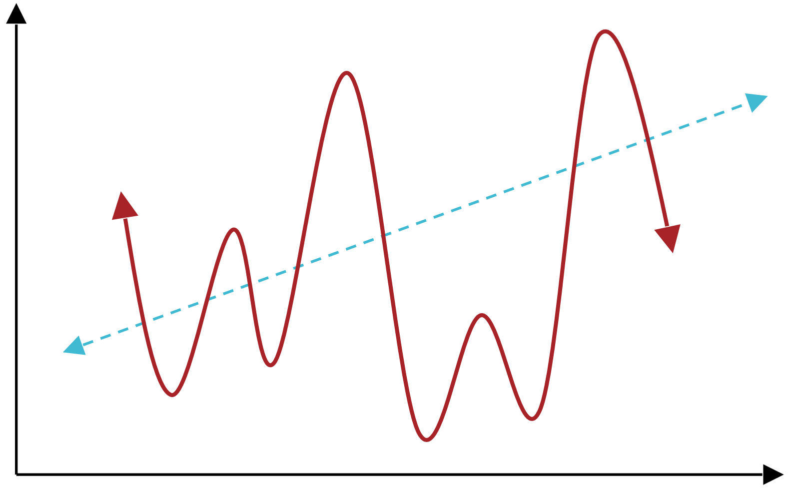
Each local minimum is a global minimum!

Convexity: local and global minima



Convex functions:

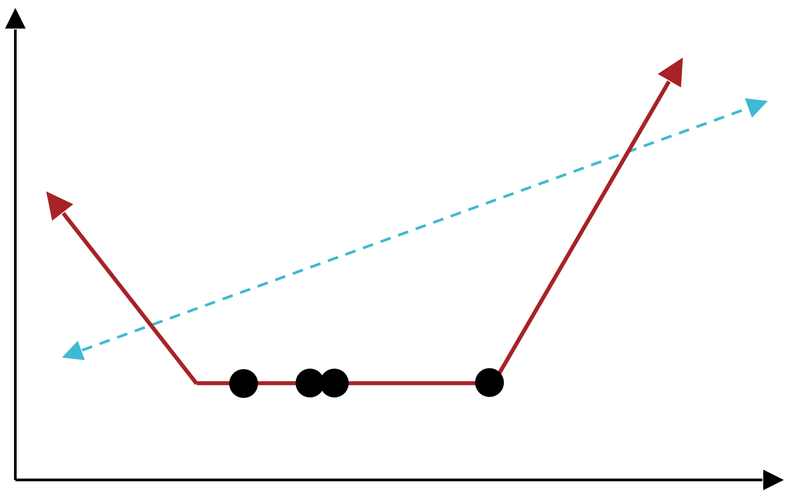
Each local minimum is a global minimum!



Non-convex functions:

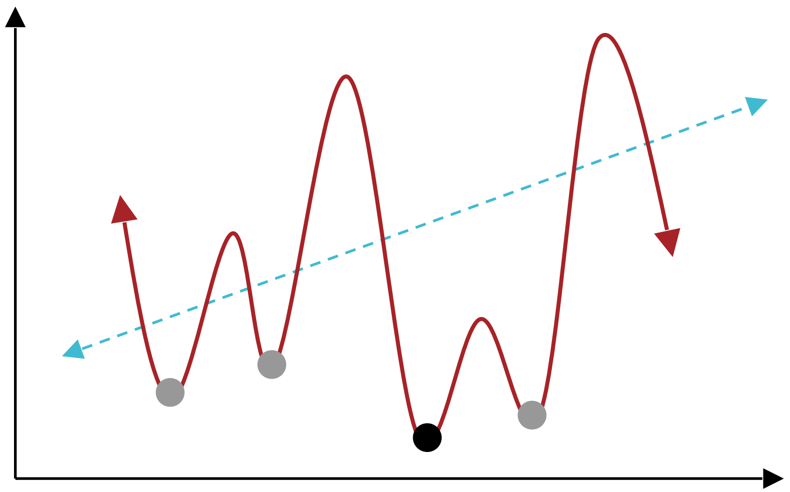
A local minimum may or may not be a global minimum…

Convexity: local and global minima



Convex functions:

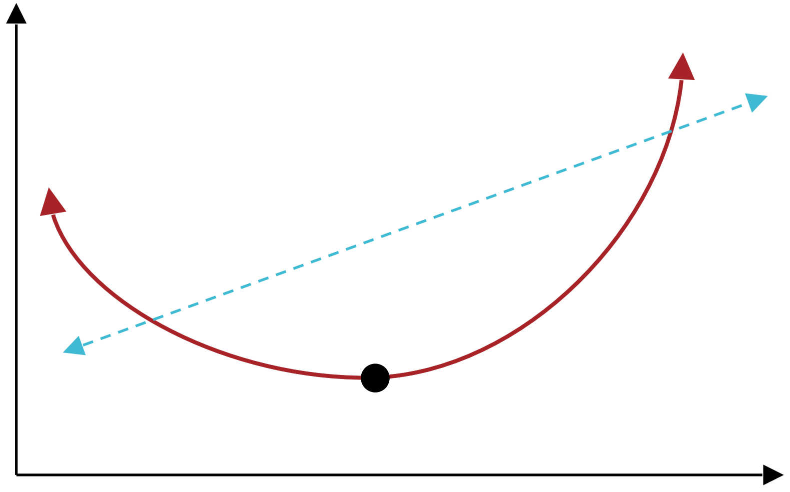
Each local minimum is a global minimum!



Non-convex functions:

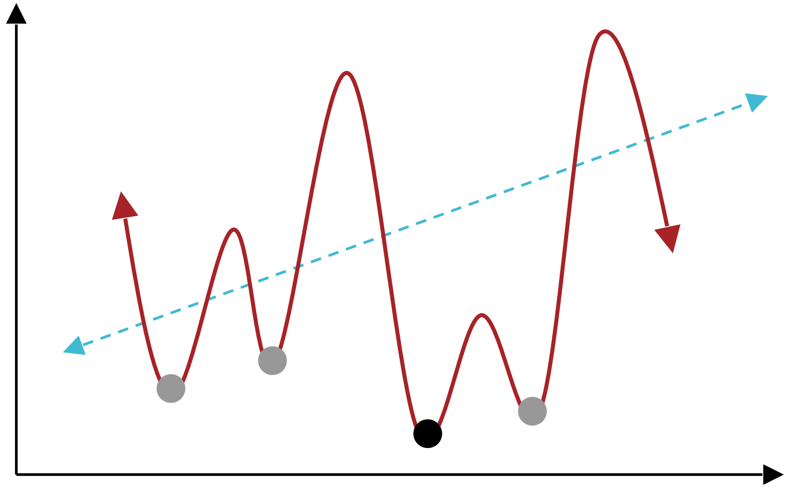
A local minimum may or may not be a global minimum…

Convexity: local and global minima



Strictly convex functions:

There exists a unique global minimum!

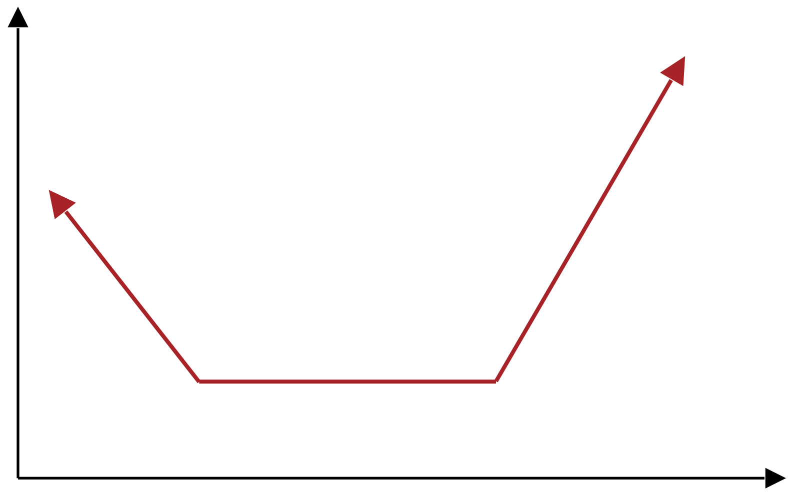


Non-convex functions:

A local minimum may or may not be a global minimum…

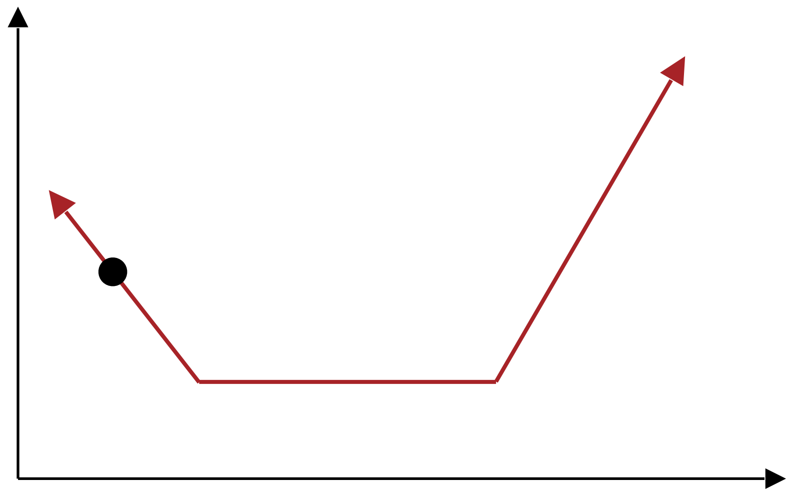
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
    - Works great if the objective function is convex!



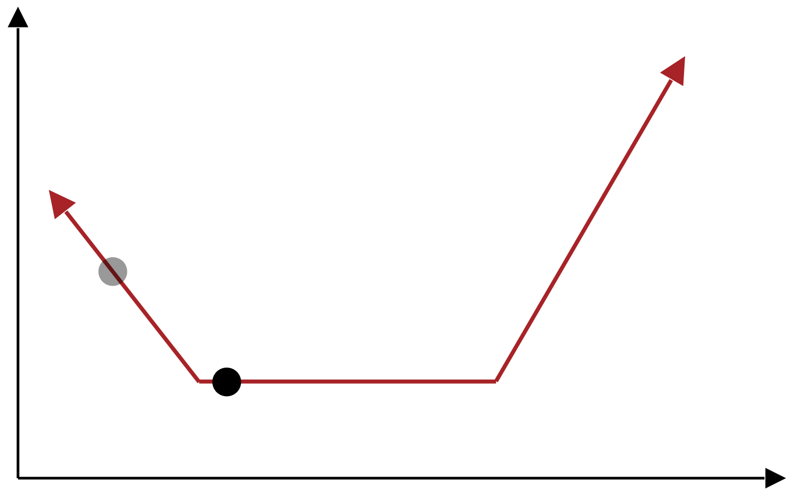
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



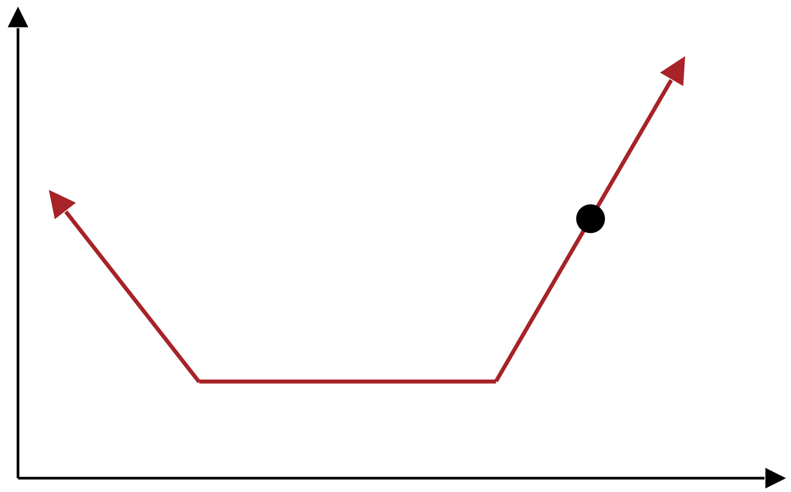
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



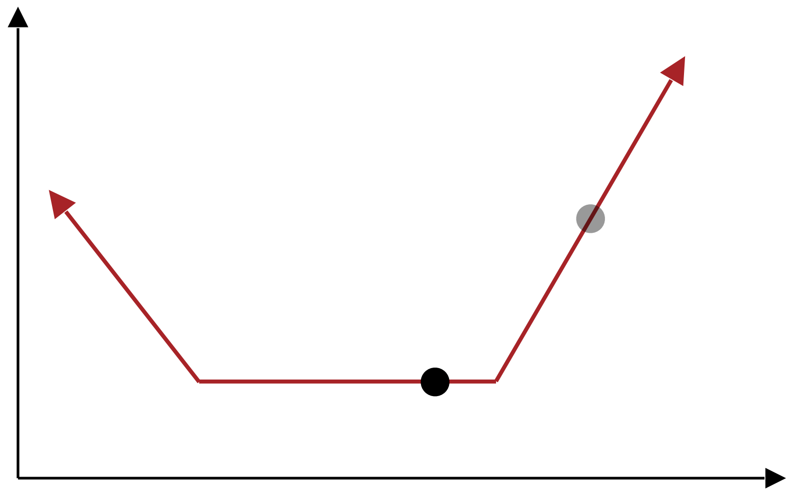
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



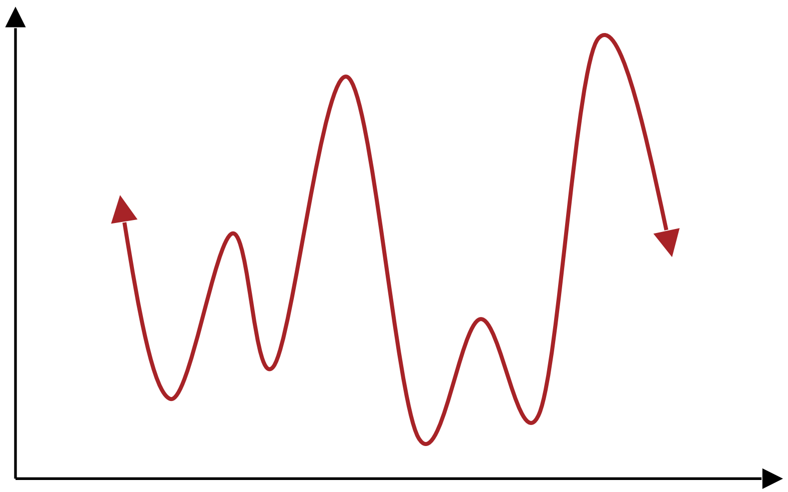
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Works great if the objective function is convex!



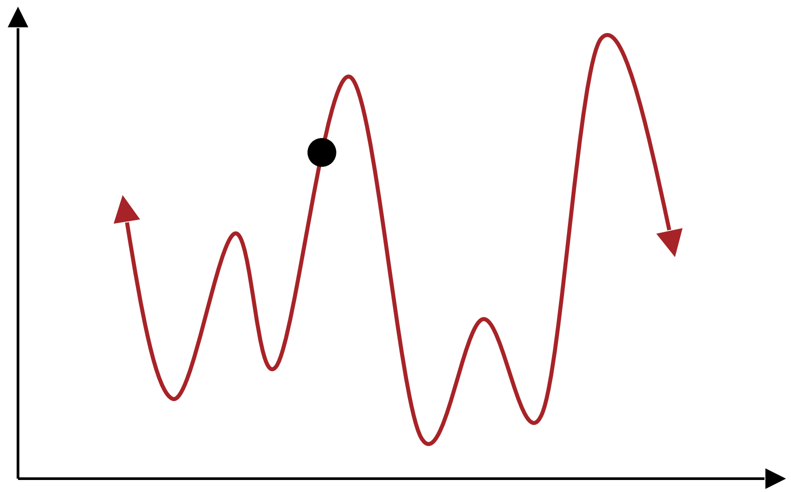
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



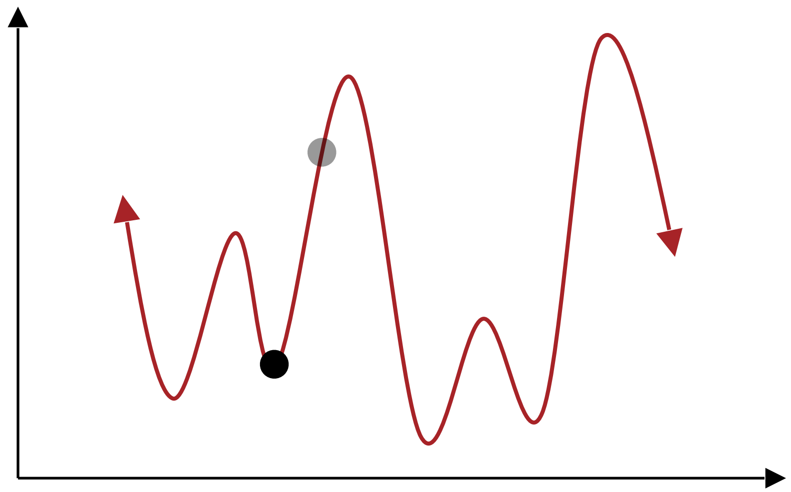
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



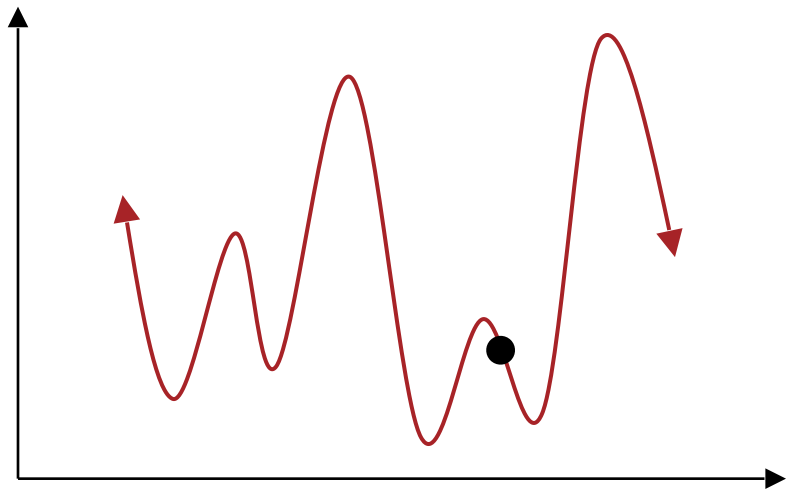
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



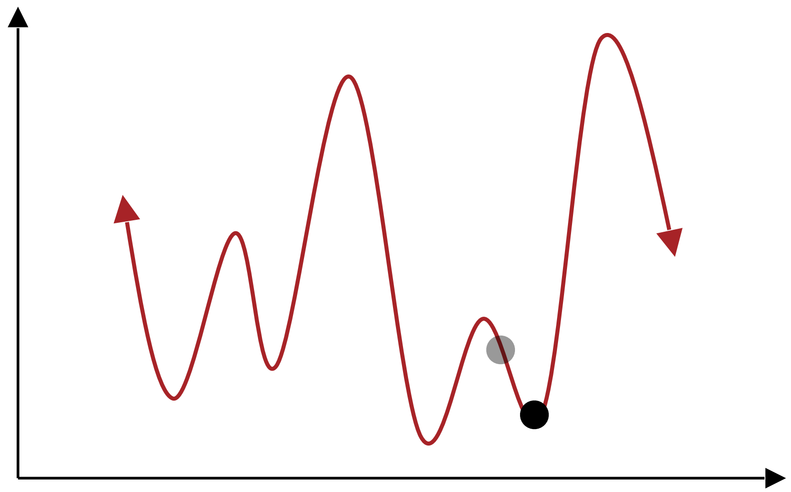
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…



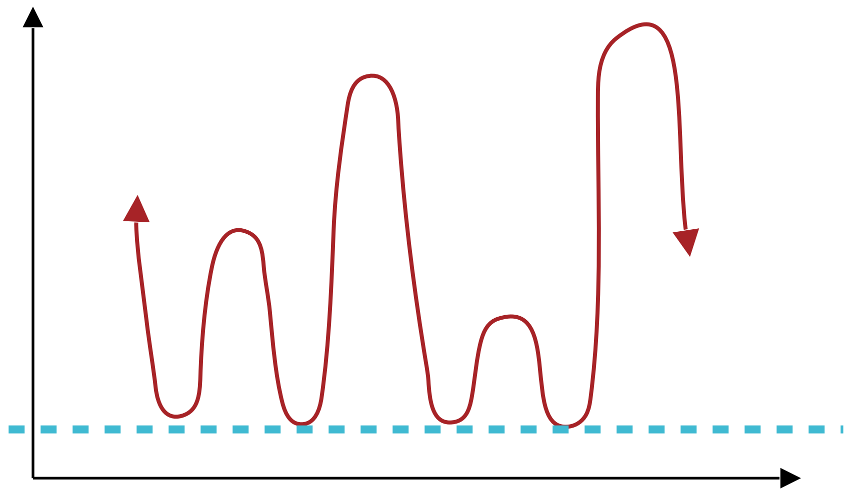
Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - Not ideal if the objective function is non-convex…

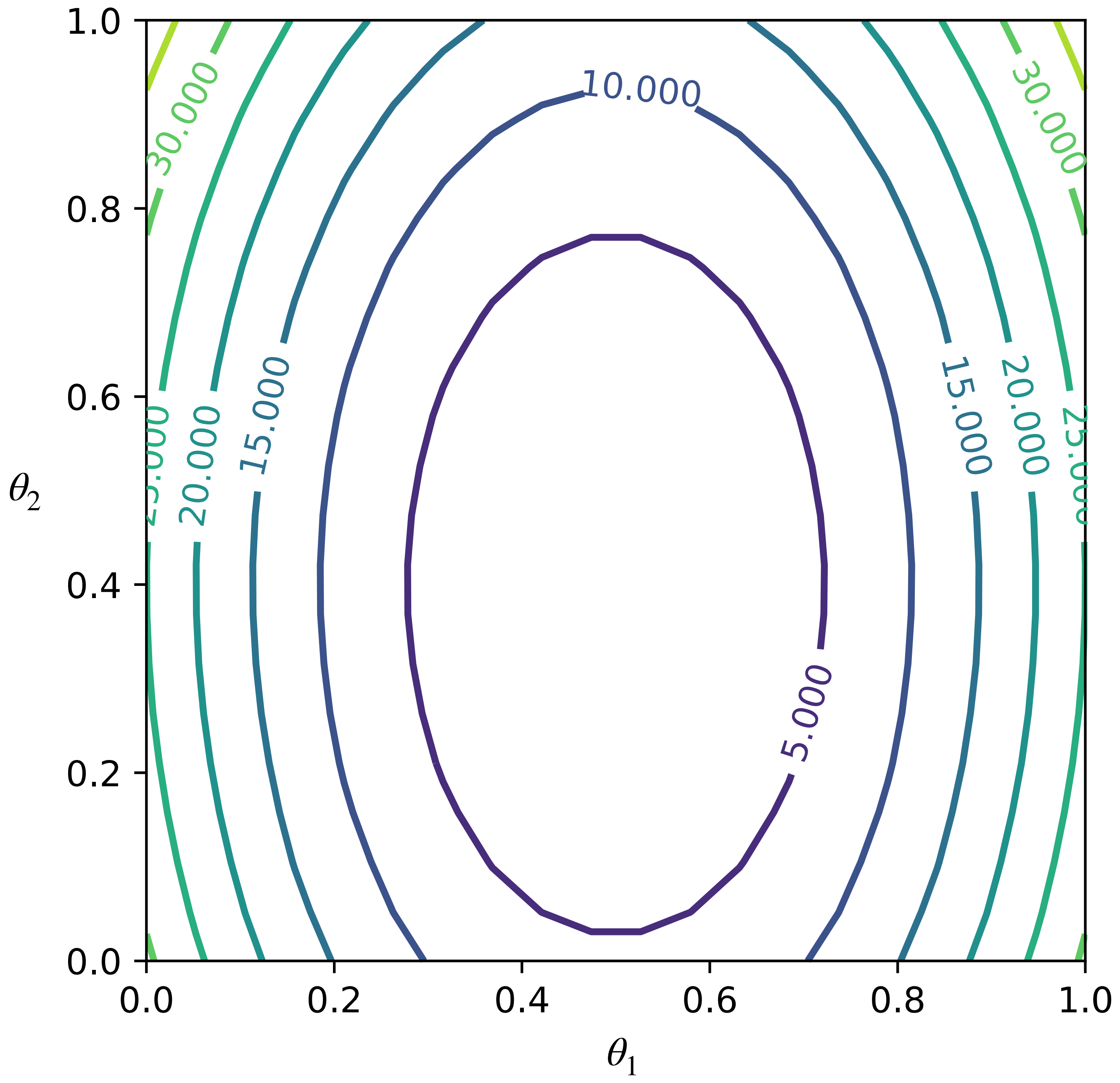


Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm – it will converge to a local minimum (if it converges)
  - But can be OK if ∃ lots of pretty good local optima

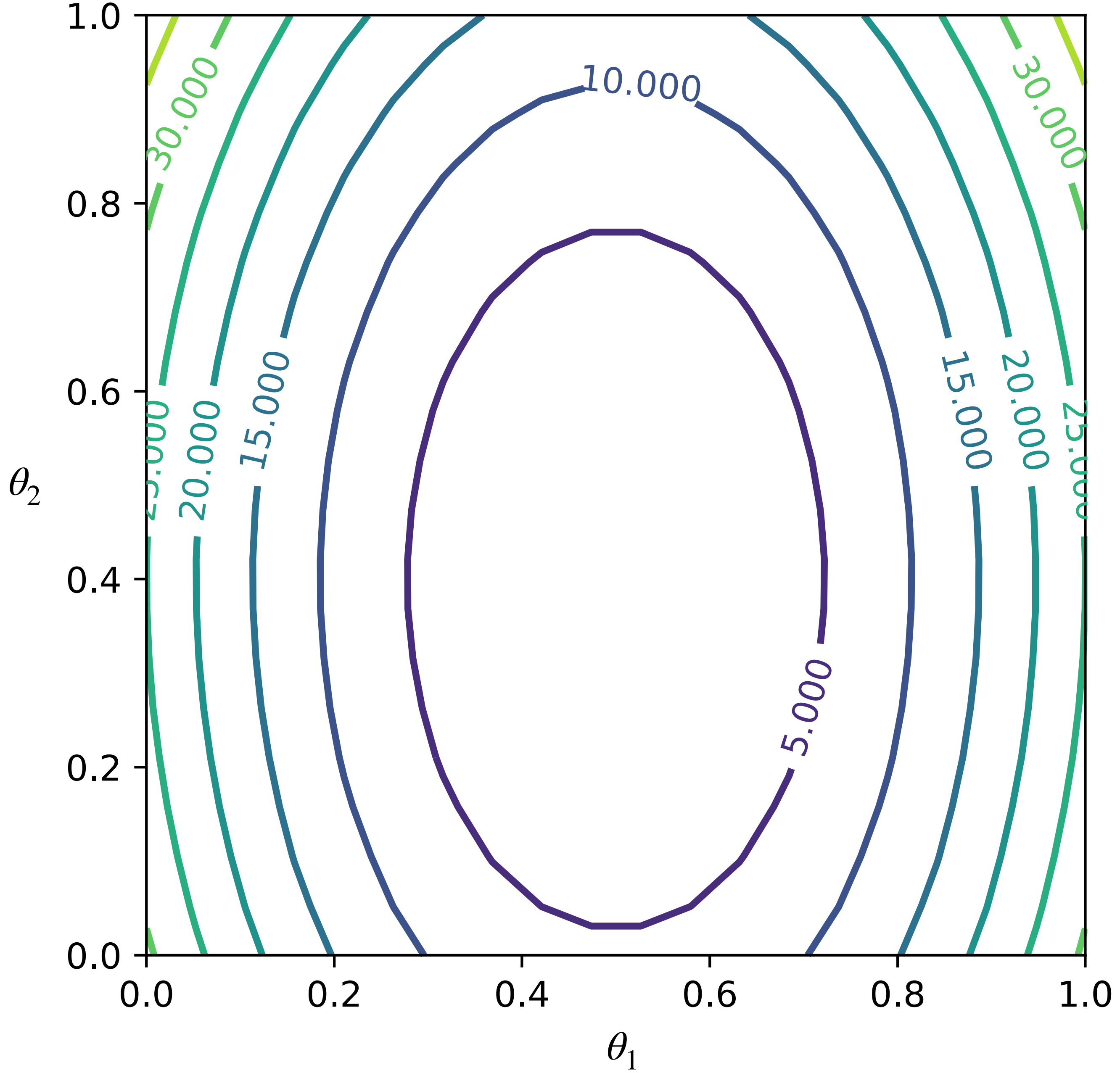


Gradient descent for linear regression: MSE is convex!



Gradient descent for linear regression: MSE is convex!

but not always strictly convex (see below for example)



OK, but calculus class told me a different way to find optima

- Set $\nabla J(\theta) = 0$ and solve for θ
  - 1D: find *critical points*
  - higher D, same idea: critical point $\leftrightarrow$ tangent is flat
- Not all critical points are local optima in general, but in our case J is convex!

Closed Form Optimization

- Notation: given training data $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$

$$X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^T} \\ 1 & \boldsymbol{x}^{(2)^T} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^T} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_D^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_D^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \cdots & x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D+1}$$

is the *design matrix*

$\boldsymbol{y} = \left[y^{(1)}, \ldots, y^{(N)}\right]^T \in \mathbb{R}^N$ is the *target vector*

Minimizing the Mean Squared Error

$$J(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}\left(y^{(i)} - \boldsymbol{\theta}^T\boldsymbol{x}^{(i)}\right)^2 = \frac{1}{2N}\sum_{i=1}^{N}\left(\boldsymbol{x}^{(i)T}\boldsymbol{\theta} - y^{(i)}\right)^2$$

$$X^\top X\theta = X^\top y$$ ← the ***normal equations***

Finding the optimal θ

- Does a solution even exist?
- Is it unique?
- If not, which one?
- How expensive is it to find desired solution?

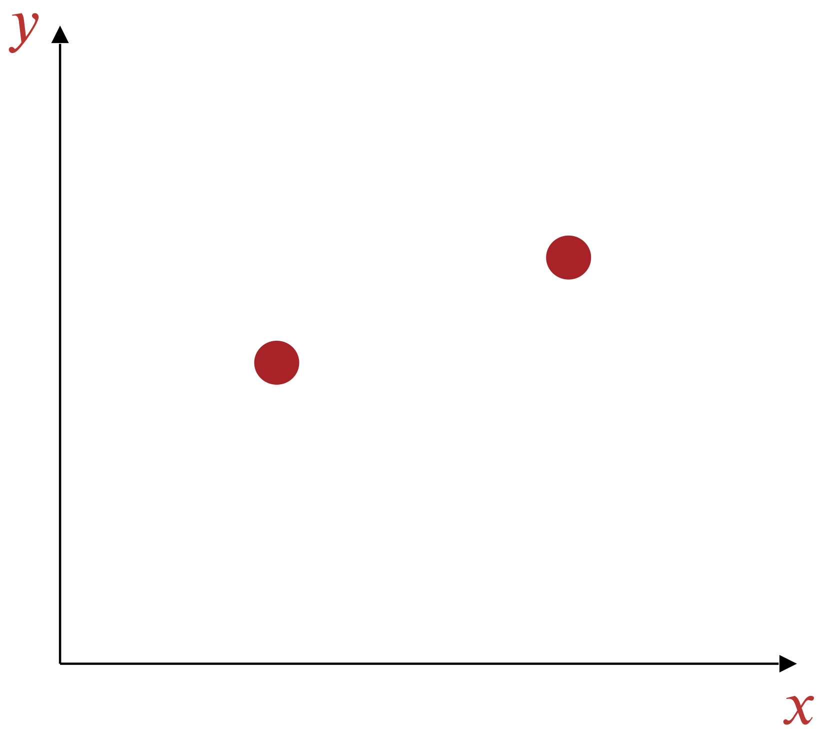
$$X^\top X\theta = X^\top y$$ ← the ***normal equations***

Finding the optimal θ

- I just want to find the solution, what should I call?
  - Options (all in `numpy.linalg`):
    - `inv(X.T @ X) @ (X.T @ y)`
    - `pinv(X.T @ X) @ (X.T @ y)`
    - `solve(X.T @ X, X.T @ y)`
    - `lstsq(X.T @ X, X.T @ y)`
    - `lstsq(X, y)`

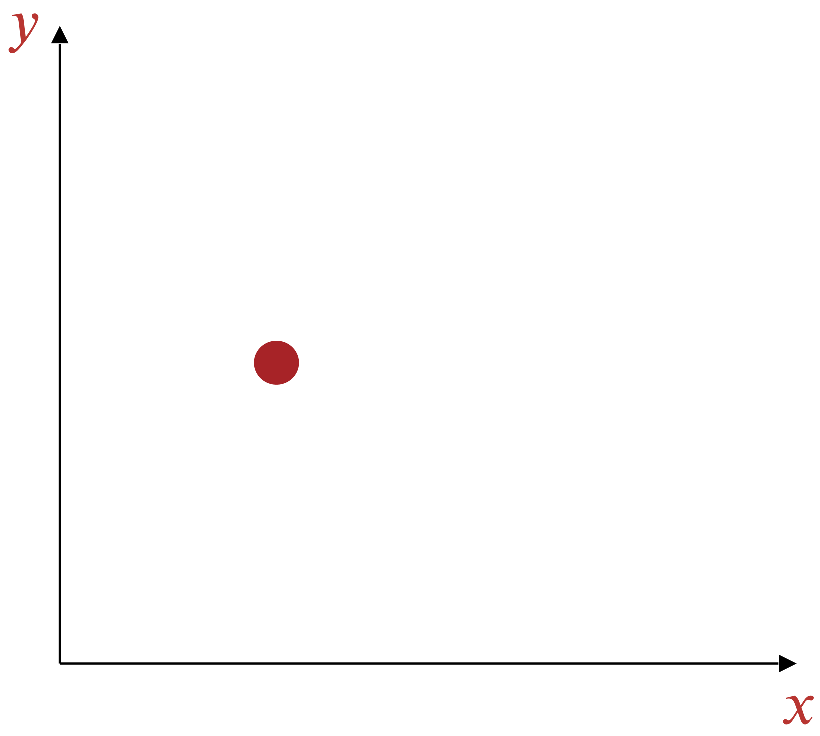
Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



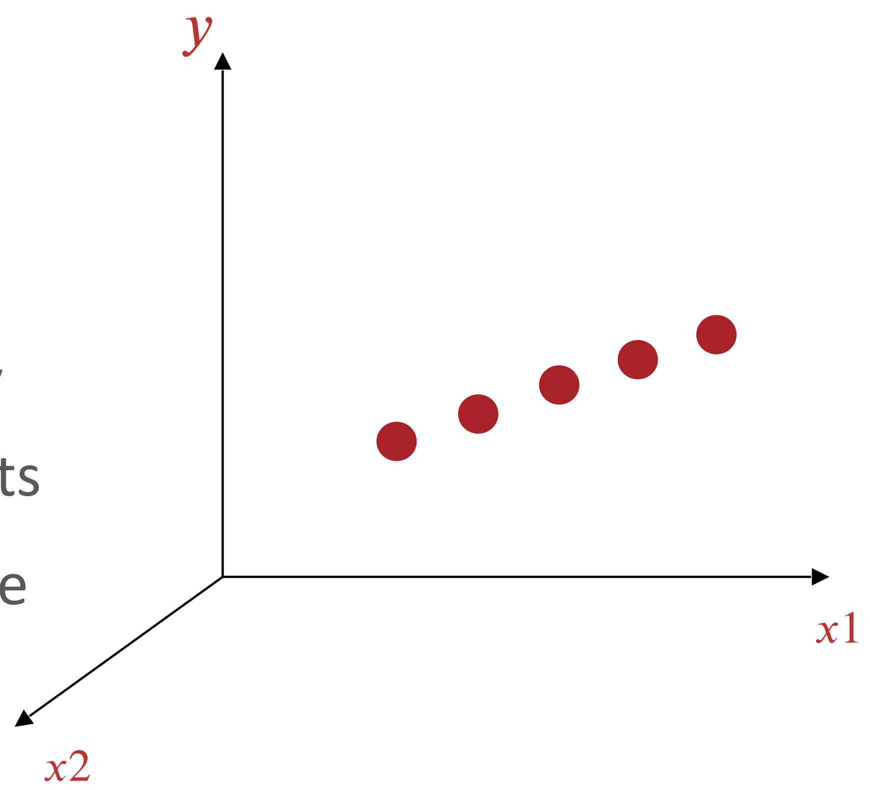
Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



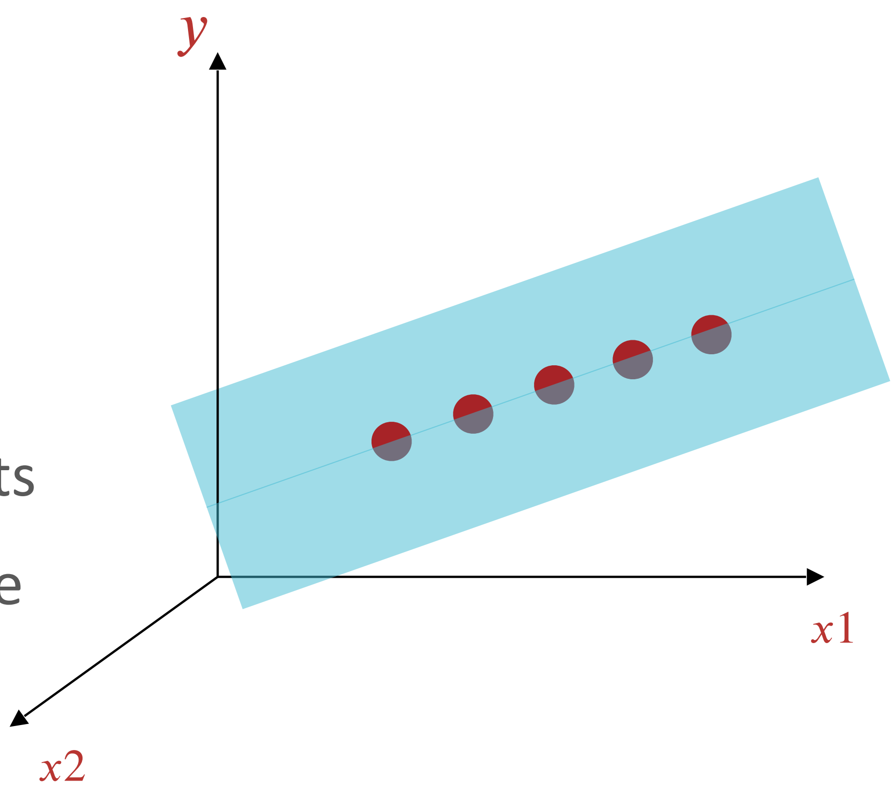
Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



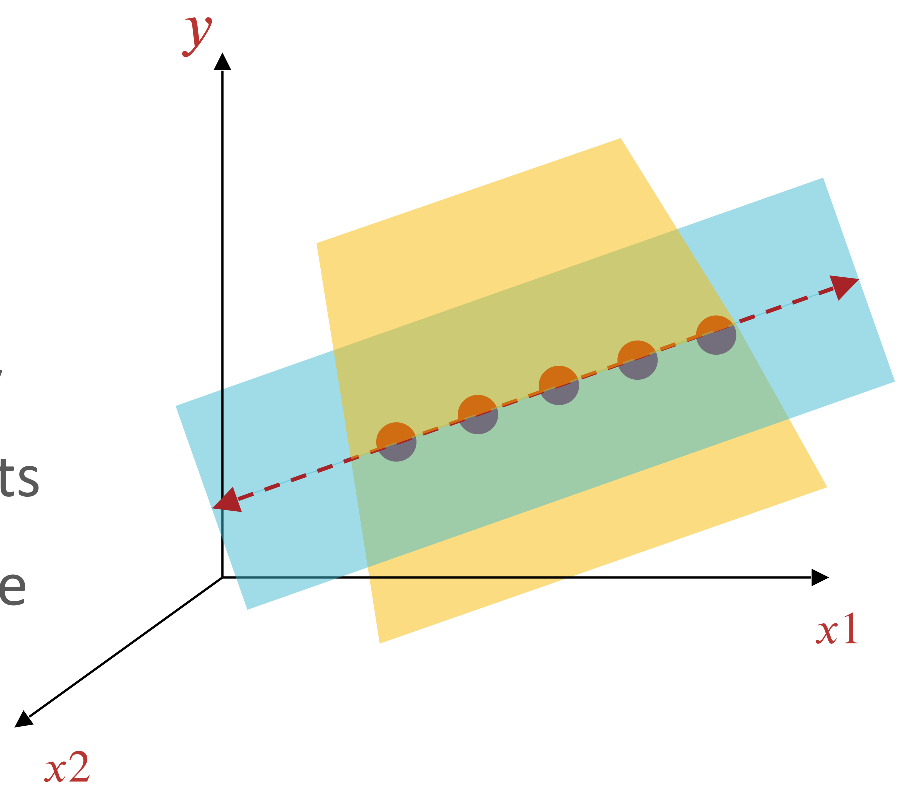
Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



Linearly independent features

- Solution is unique if number of examples N is *at least as large* as number of *linearly independent* features
  - independent = not a linear function of other features
  - e.g., $x_1^{(i)}$ = length (mm) and $x_2^{(i)}$ = length (inches): *not* linearly independent
  - e.g., if examples are on a line in 2d, number of linearly independent features = 1 (not 2)
  - e.g., on a line or plane in 3d: 1 or 2, not 3
  - etc.
- Can drop features to get independence, or resolve ambiguity by picking minimum norm solution

Recap: exact vs. gradient descent

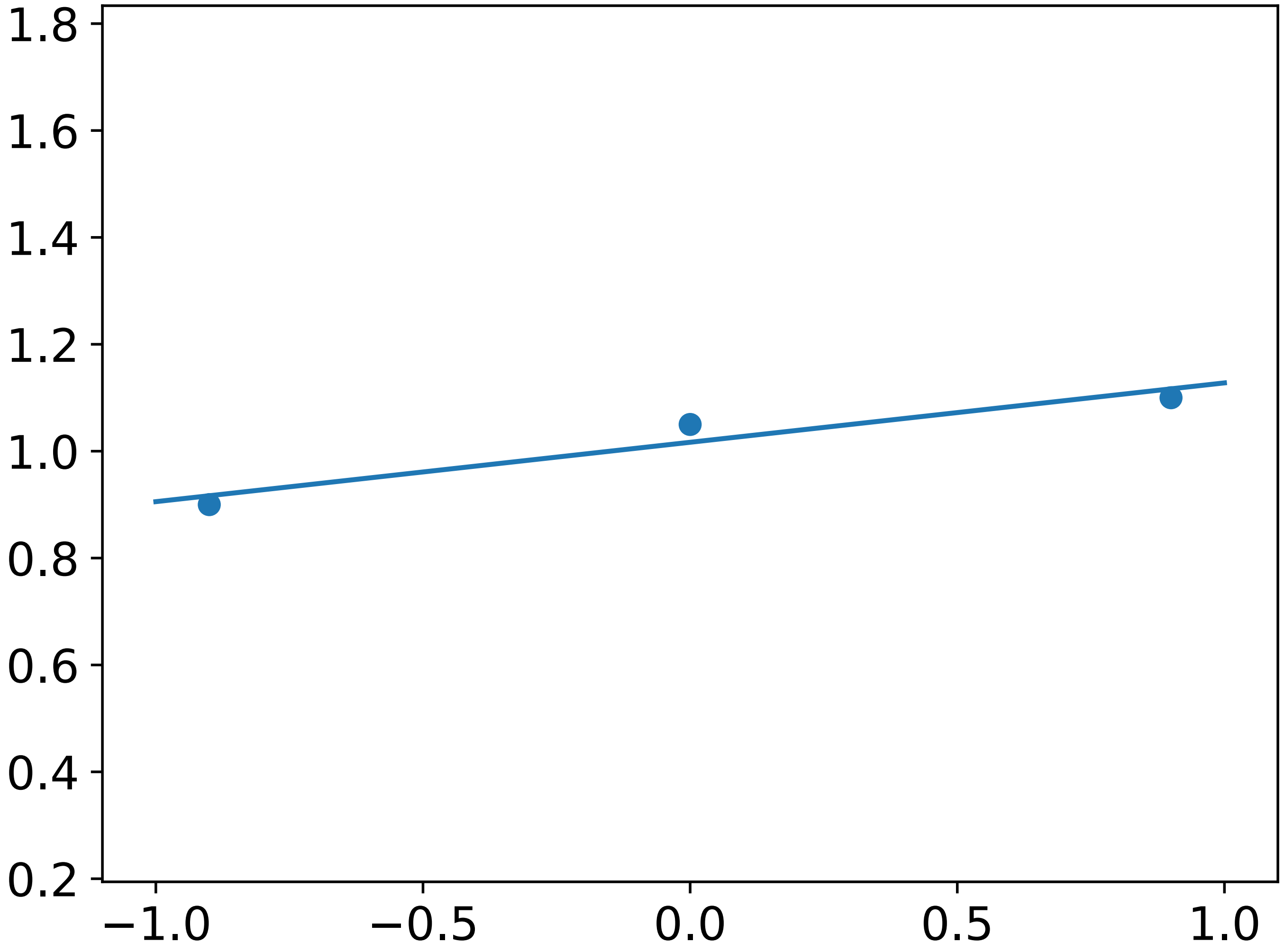
- Use *exact solution* if M is small and N is large
  - fast enough since M is small, accurate solution is worth it since N is large
- Use (variants of) *gradient descent* if M is large
- If M and N both small, both methods are OK

Linear Regression Learning Objectives

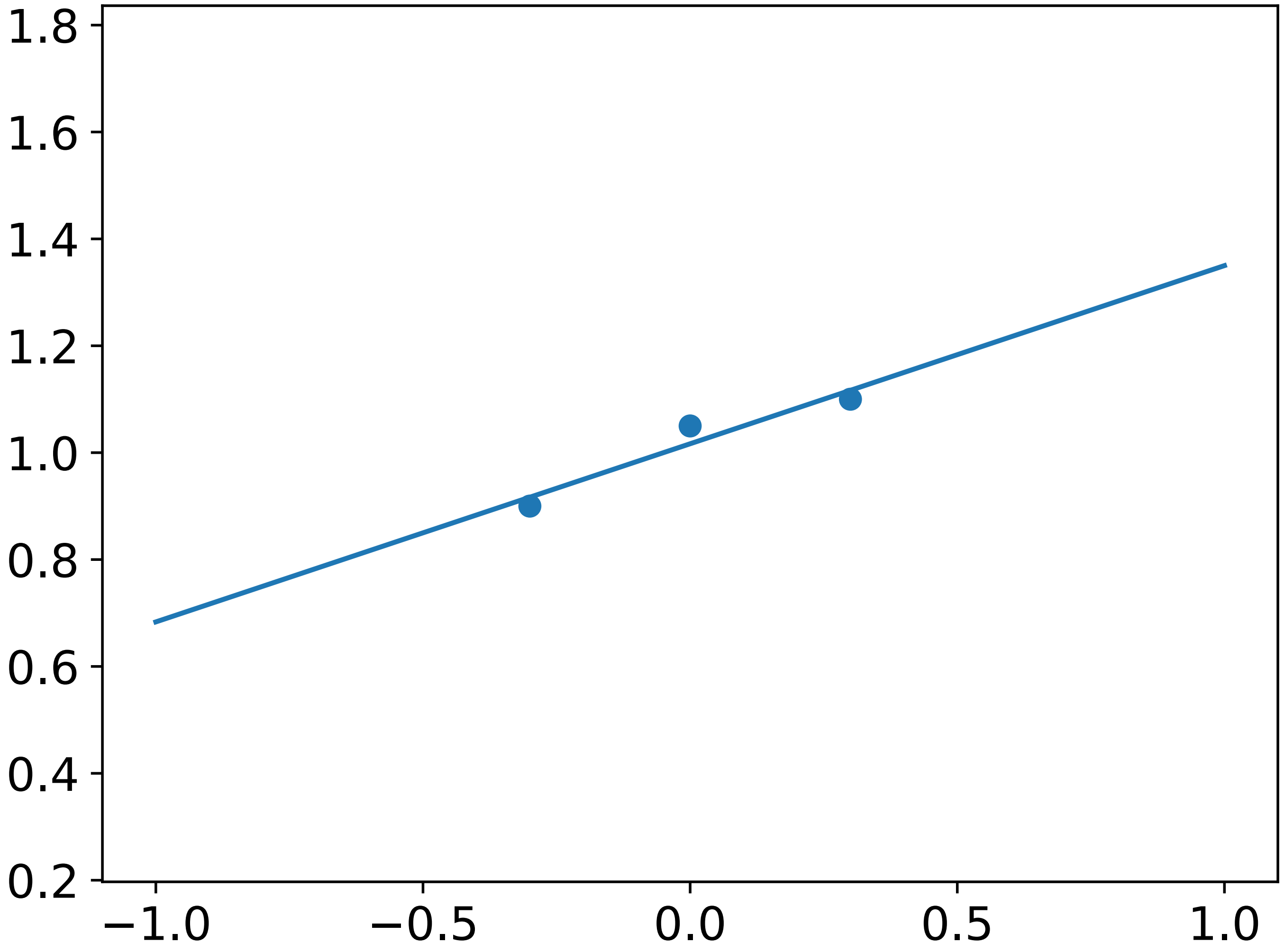
You should be able to…

- Design k-NN Regression and Decision Tree Regression
- Choose a Linear Regression optimization technique that is appropriate for a particular dataset by analyzing the tradeoff of computational complexity vs. convergence speed
- Implement learning for Linear Regression using gradient descent or closed form optimization (with well chosen NumPy calls!)
- Identify situations where least squares regression has exactly one solution or infinitely many solutions

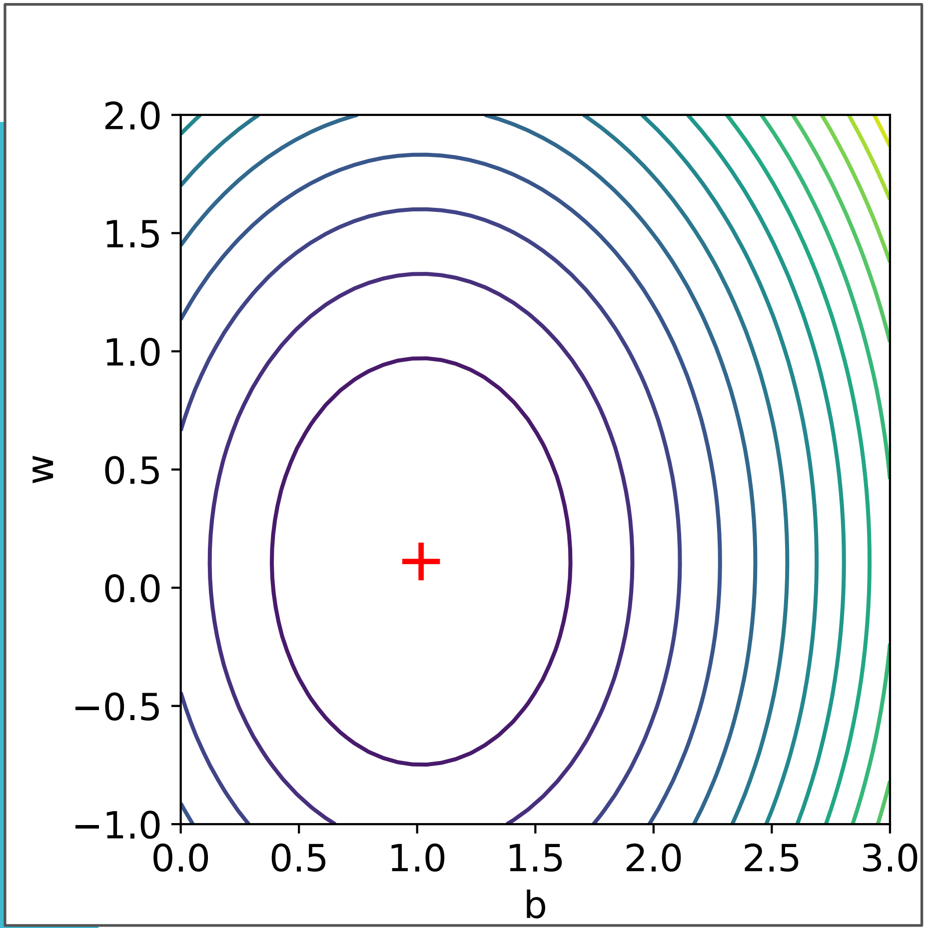
A tale of two datasets



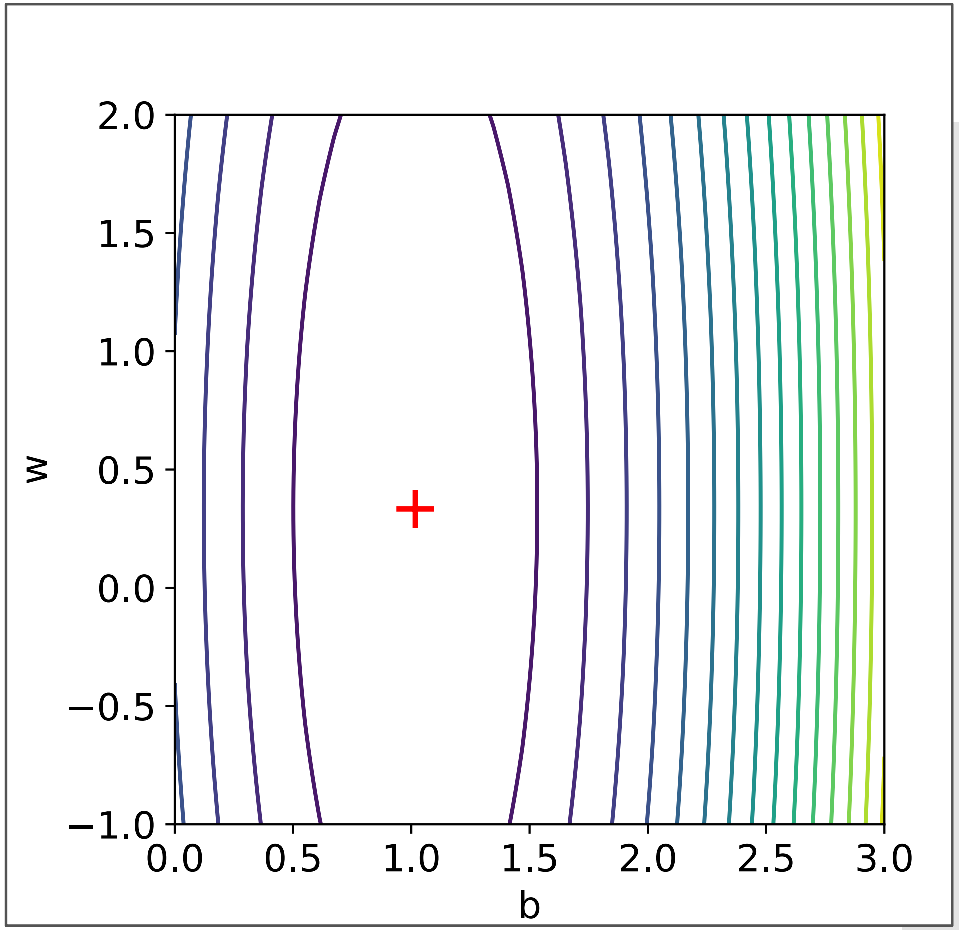
A tale of two datasets



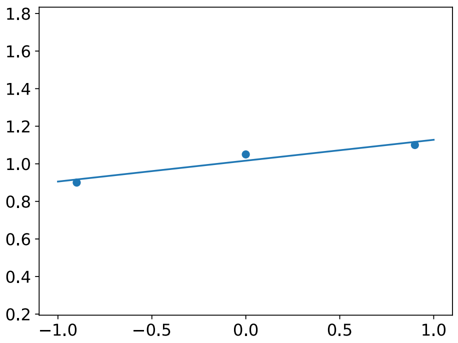
MSE loss



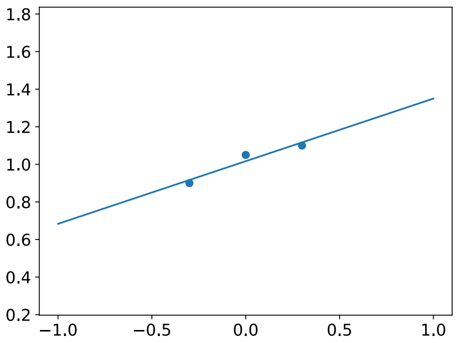
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
w
0.0 0.5 1.0 1.5 2.0 2.5 3.0
b



2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
w
0.0 0.5 1.0 1.5 2.0 2.5 3.0
b

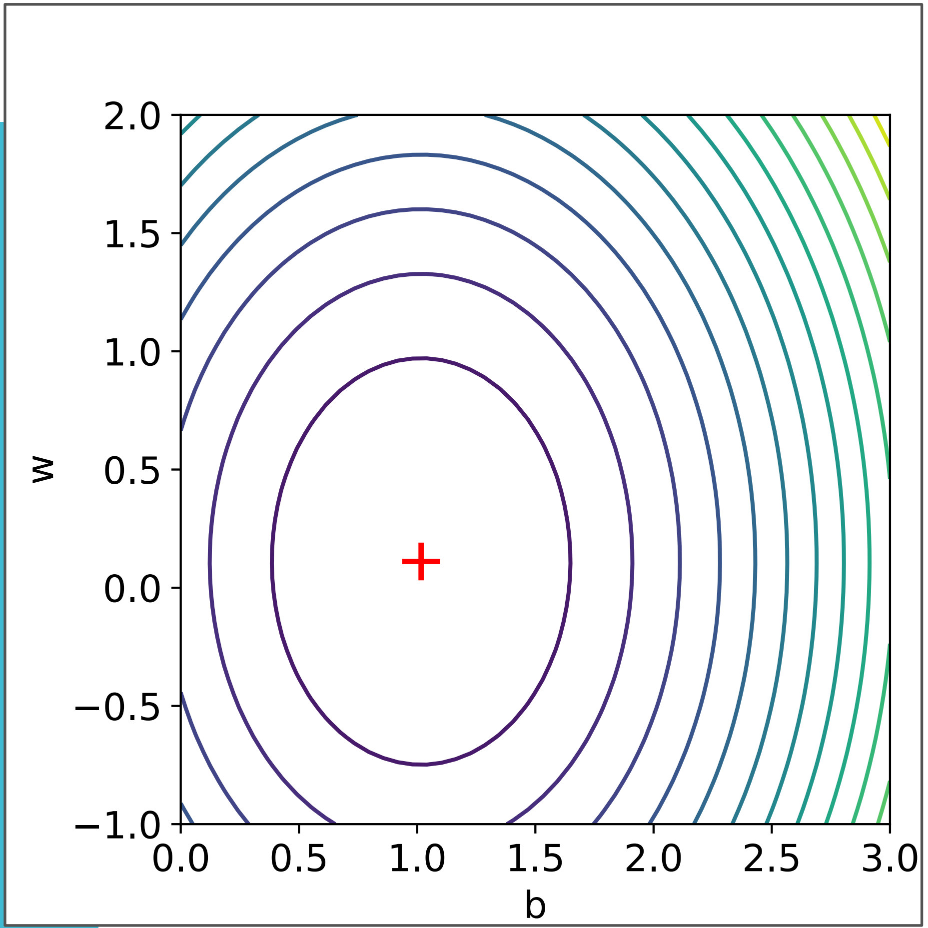


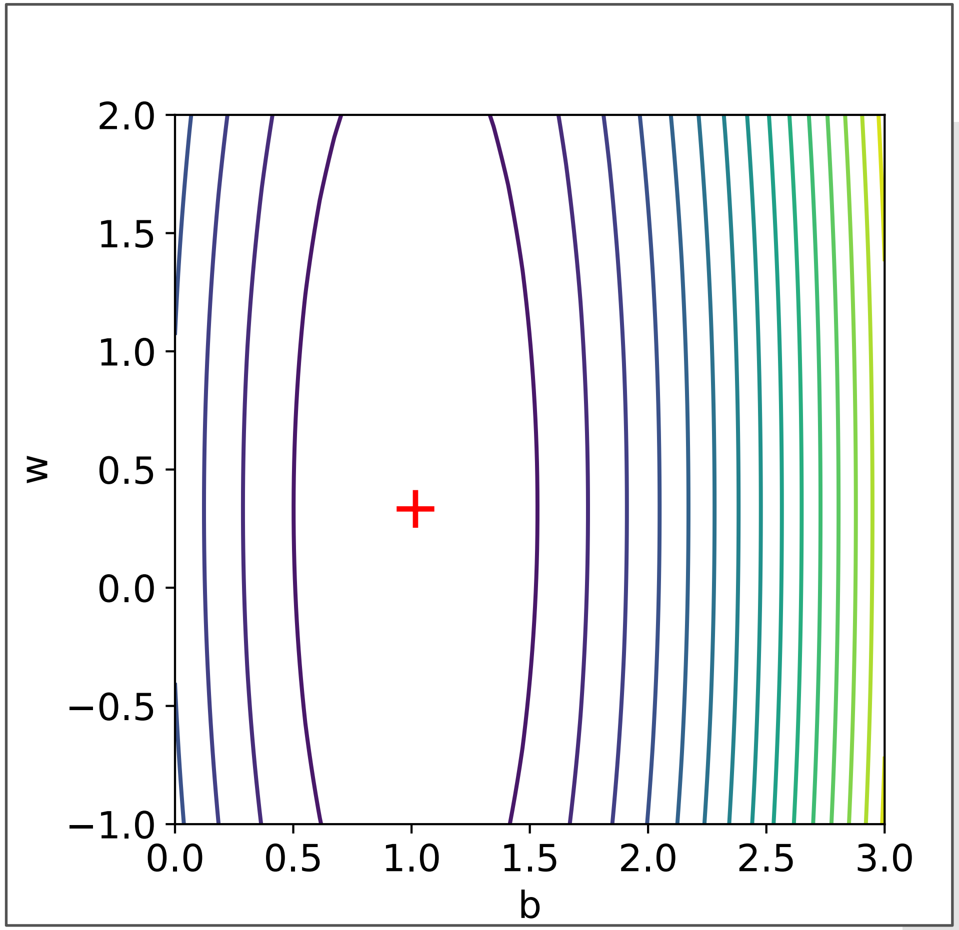
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
−1.0 −0.5 0.0 0.5 1.0

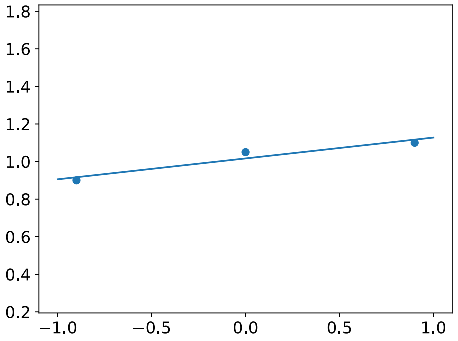


1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
−1.0 −0.5 0.0 0.5 1.0

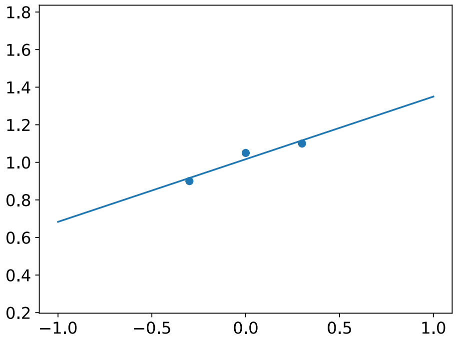
MSE loss





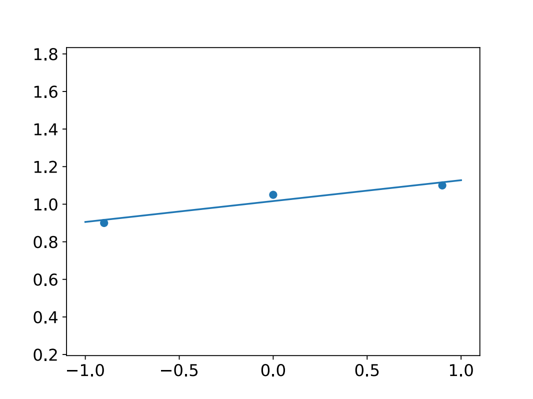


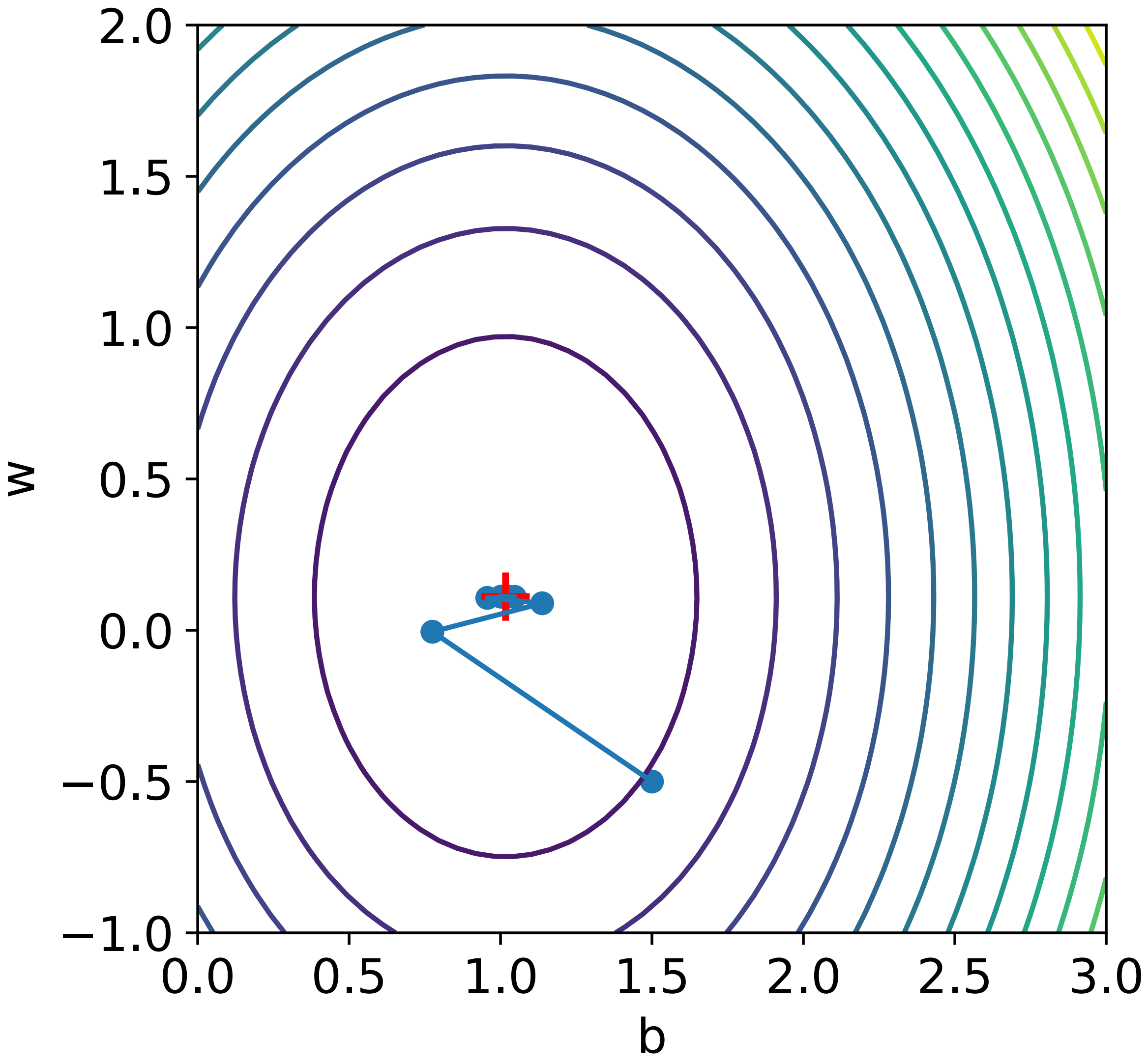
well conditioned



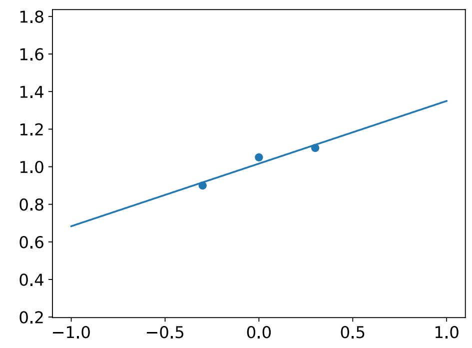
poorly conditioned

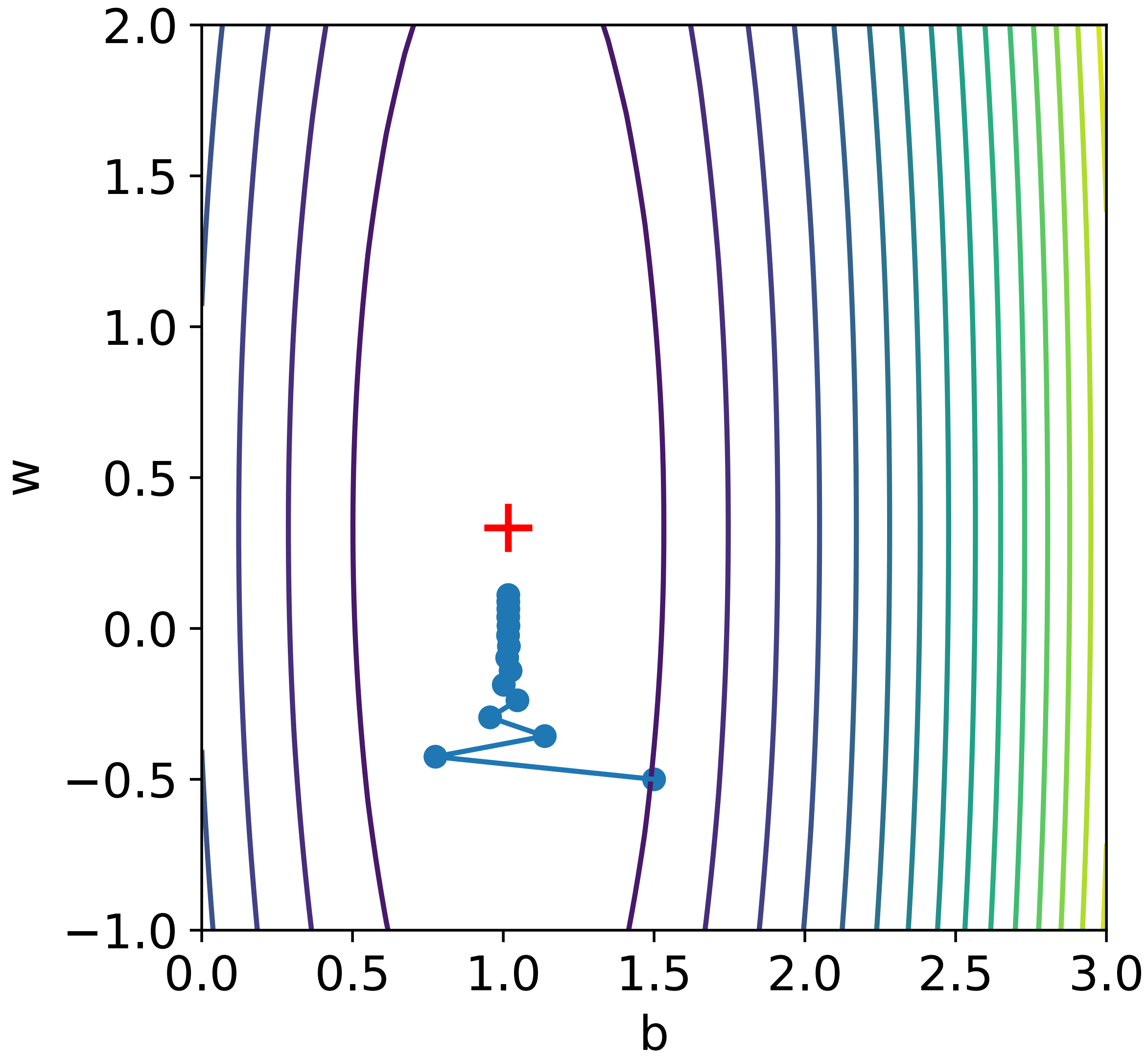
Gradient descent (good conditioning)



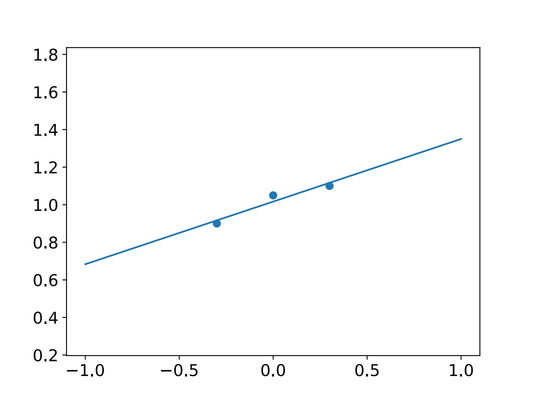


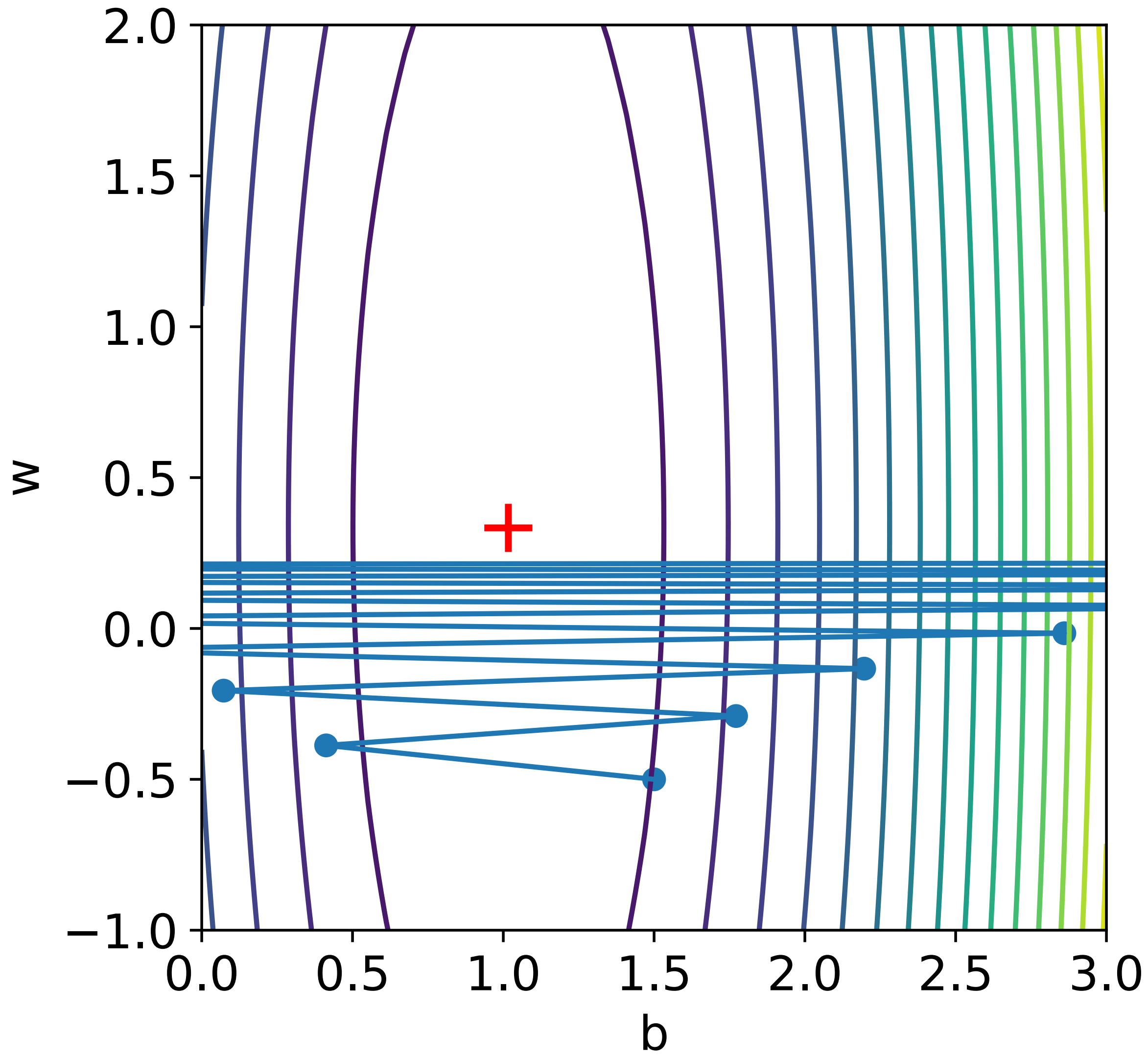
Gradient descent (poor conditioning)





Gradient descent (poor conditioning)





What could we do?

- For horizontal direction (b), want a small learning rate to prevent oscillation
- For vertical direction (w), want a large learning rate to make fast enough progress
- Ideas?

What if we could discover a good scaling automatically?

- Wouldn’t it be great if we could automatically scale down the learning rate in directions where we start to oscillate?
    - then we’d be free to set learning rate high enough to make progress in other dimensions

Momentum

- Exponential moving average

if gradients always point ↑

if gradients alternate ↑ ↓

- Modified gradient descent update

Gradient descent with momentum

procedure GDLR_M$(\mathscr{D}, \boldsymbol{\theta}^{(0)}, \mathbf{g}^{(0)})$

$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}, \quad \bar{\mathbf{g}} \leftarrow \mathbf{g}^{(0)}$

while not converged do

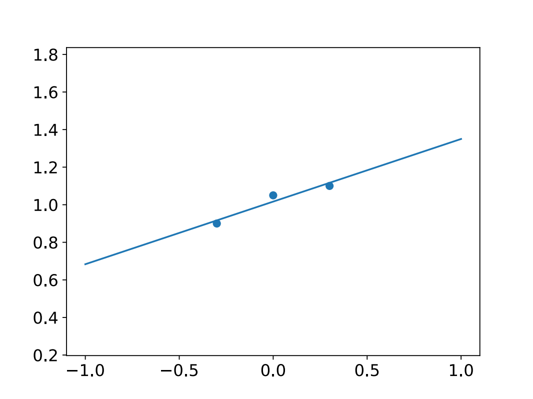
$\mathbf{g} \leftarrow \sum_{i=1}^{N} (\boldsymbol{\theta}^\top \mathbf{x}^{(i)} - \mathbf{y}^{(i)})\mathbf{x}^{(i)}$

$\bar{\mathbf{g}} \leftarrow \beta\bar{\mathbf{g}} + (1 - \beta)\mathbf{g}$

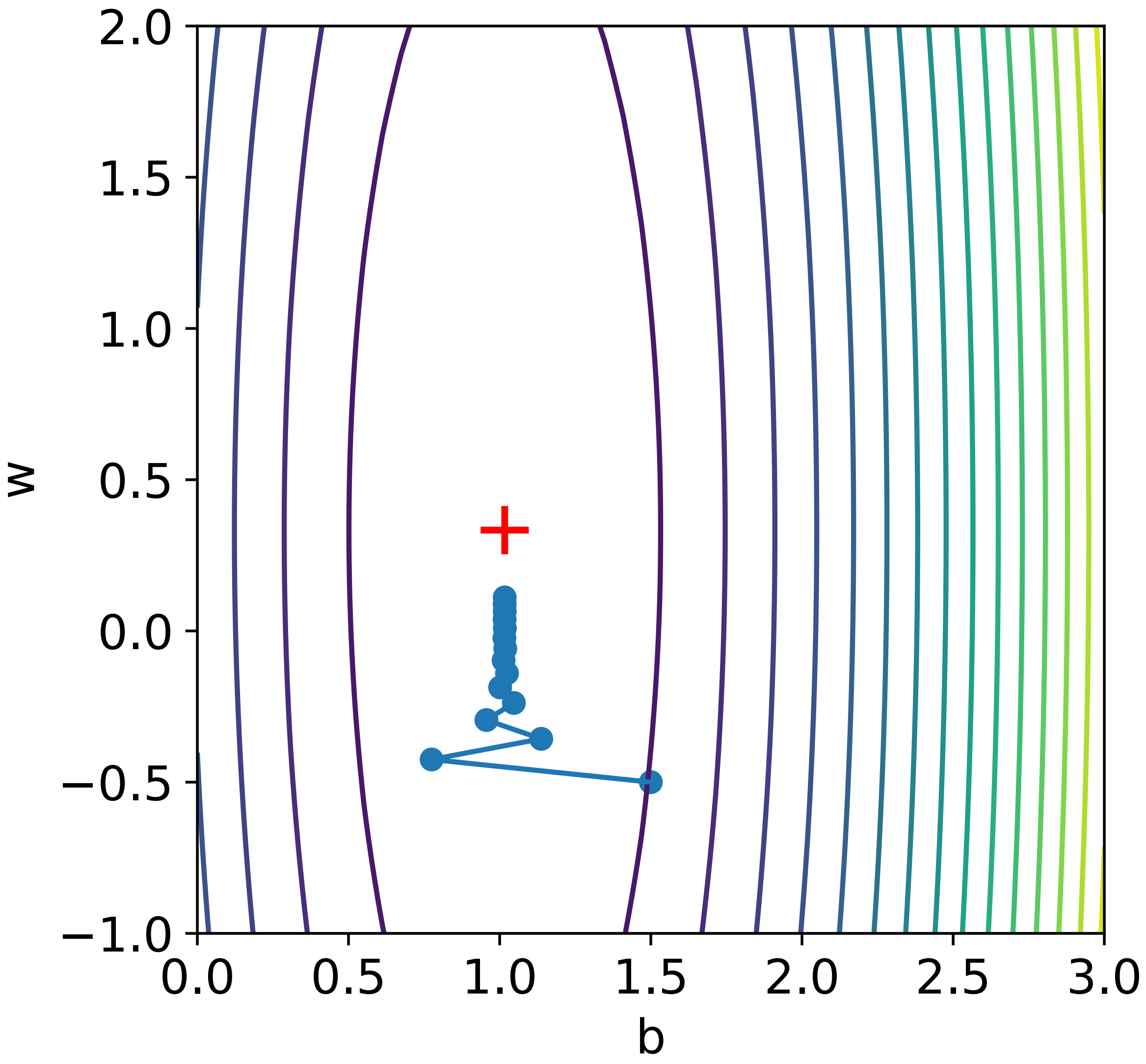
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma\bar{\mathbf{g}}$

return $\boldsymbol{\theta}$

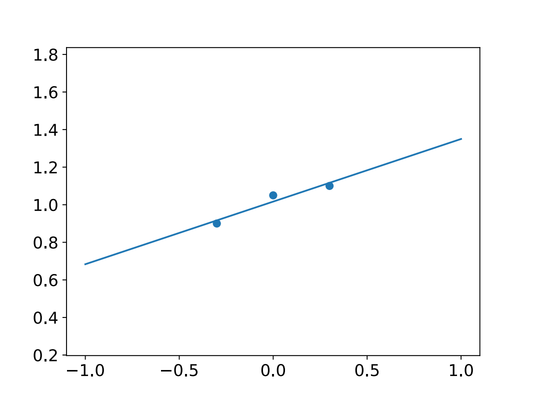
Gradient descent + momentum (poor conditioning)



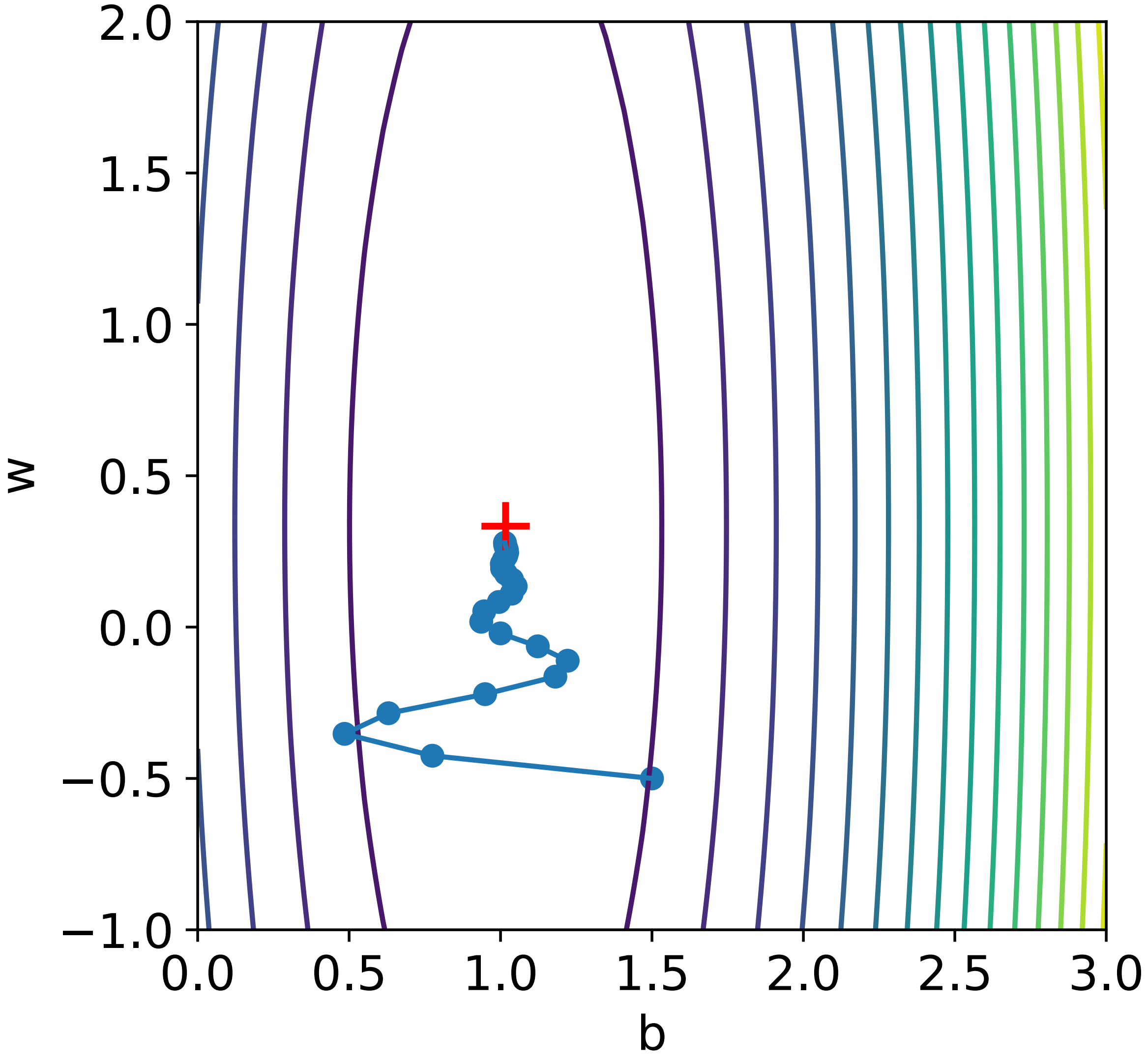
learning rate 0.5
momentum 0.0



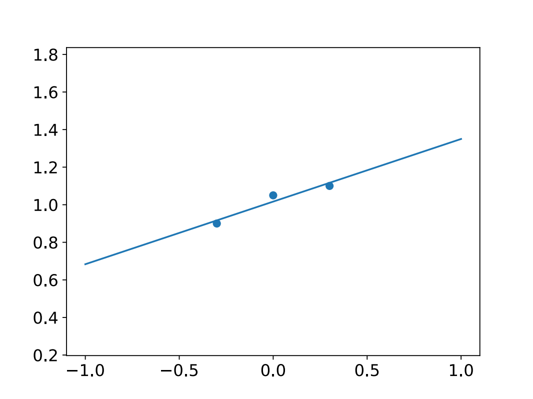
Gradient descent + momentum (poor conditioning)



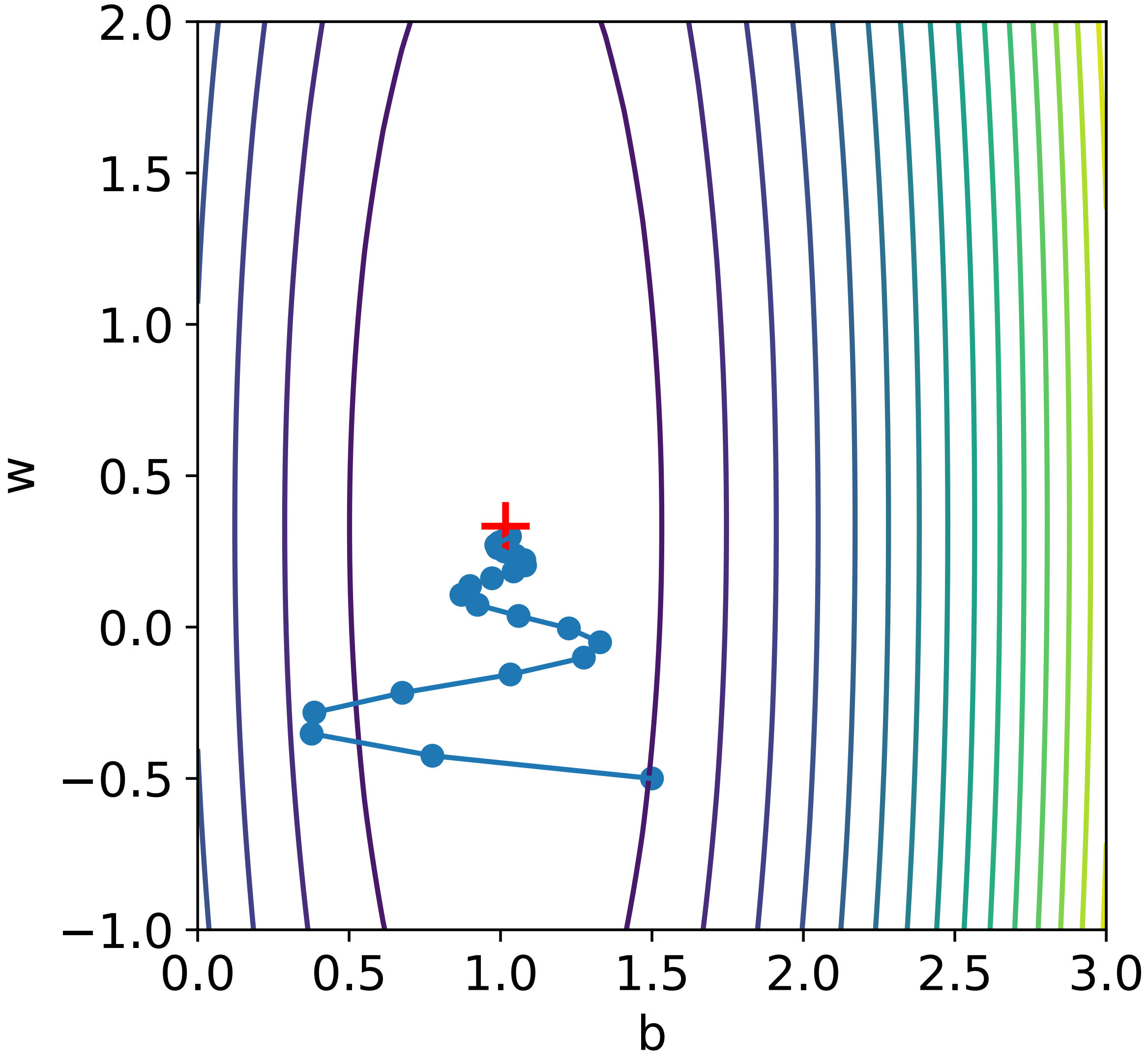
learning rate 0.5
momentum 0.6



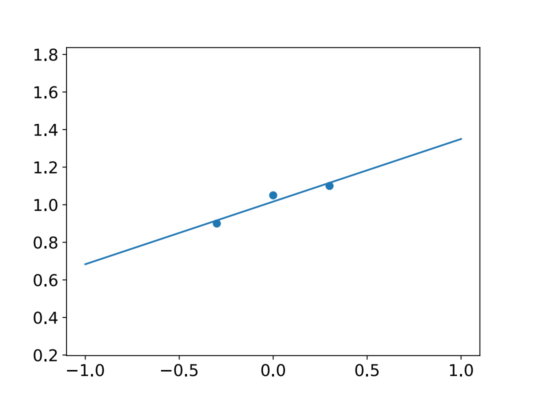
Gradient descent + momentum (poor conditioning)



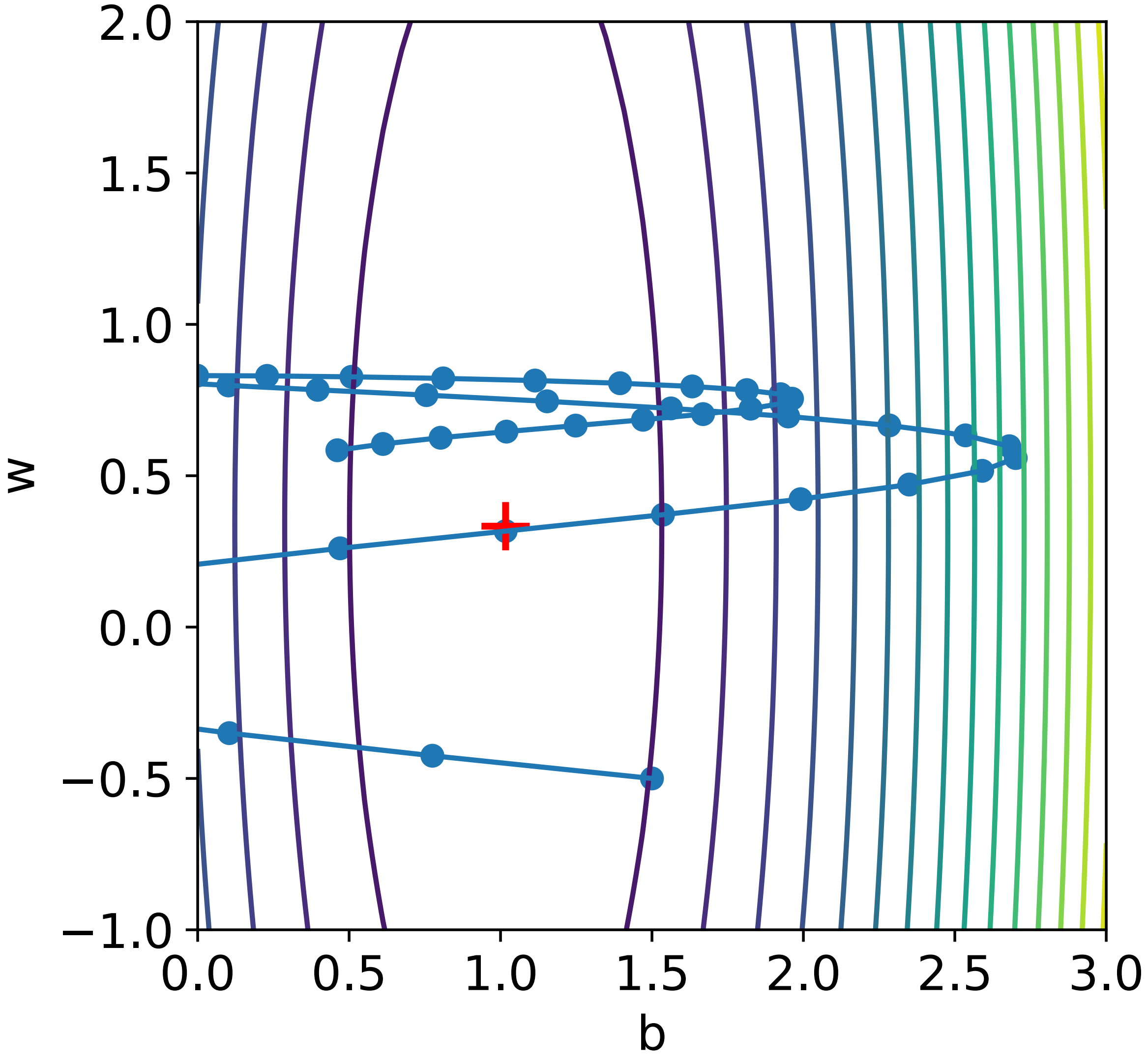
learning rate 0.5
momentum 0.7



Gradient descent + momentum (poor conditioning)



learning rate 0.5
momentum 0.95



Preview: nonconvex