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Optimization
in deep learning

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Ingredients for supervised deep learning

- A task definition
- An evaluation metric
- A large amount of high-quality labeled data (>100 000)
- A learning algorithm:
  - End-to-end differentiable computational graph
  - A gradient calculation algorithm: backpropagation
  - **A parameter optimizer**

Ingredients for supervised deep learning

- A task definition
- **An evaluation metric**: we want to maximize the model performance.
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Why optimization is important in ML?

- We want to maximize the model performance evaluated by the metric.
- Usually, the evaluation metric is not differentiable (e.g., accuracy).
- We need a differentiable surrogate function for training the model.

Objectives of the presentation

Give the intuition to the basic concepts of optimization for deep learning.

Three concepts to remember:

- Preconditioning
- Momentum
- Stochastic optimization

Global minimum

x^* is a *global minimum* of $f : \mathbb{R}^n \rightarrow \mathbb{R}$ iif

$$\forall x \in \mathbb{R}^n, f(x^*) \leq f(x)$$

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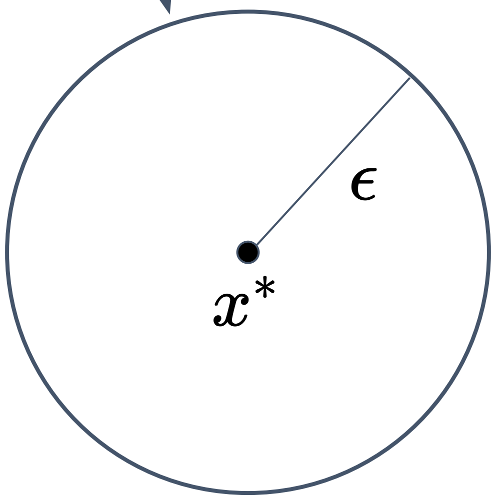
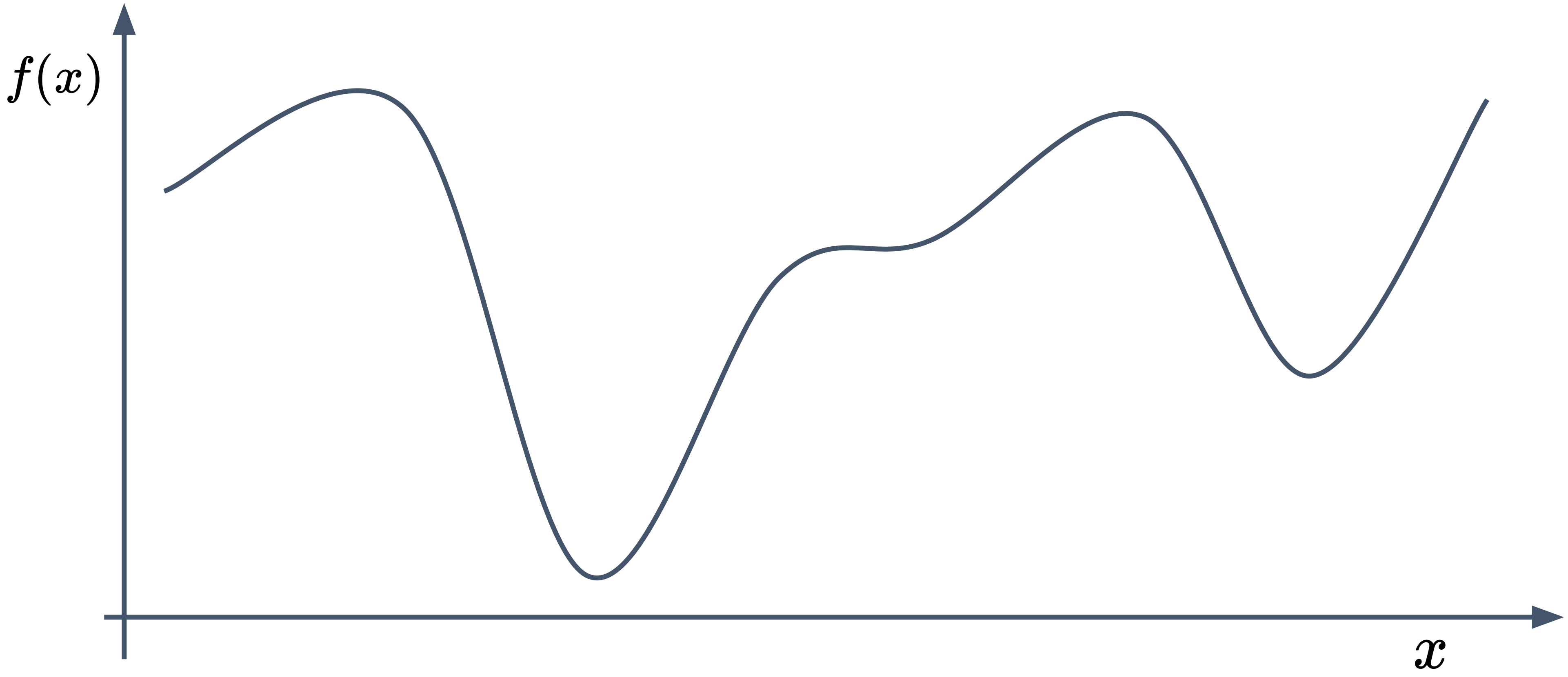
Local minimum

x^* is a *local minimum* of $f : \mathbb{R}^n \to \mathbb{R}$ iif

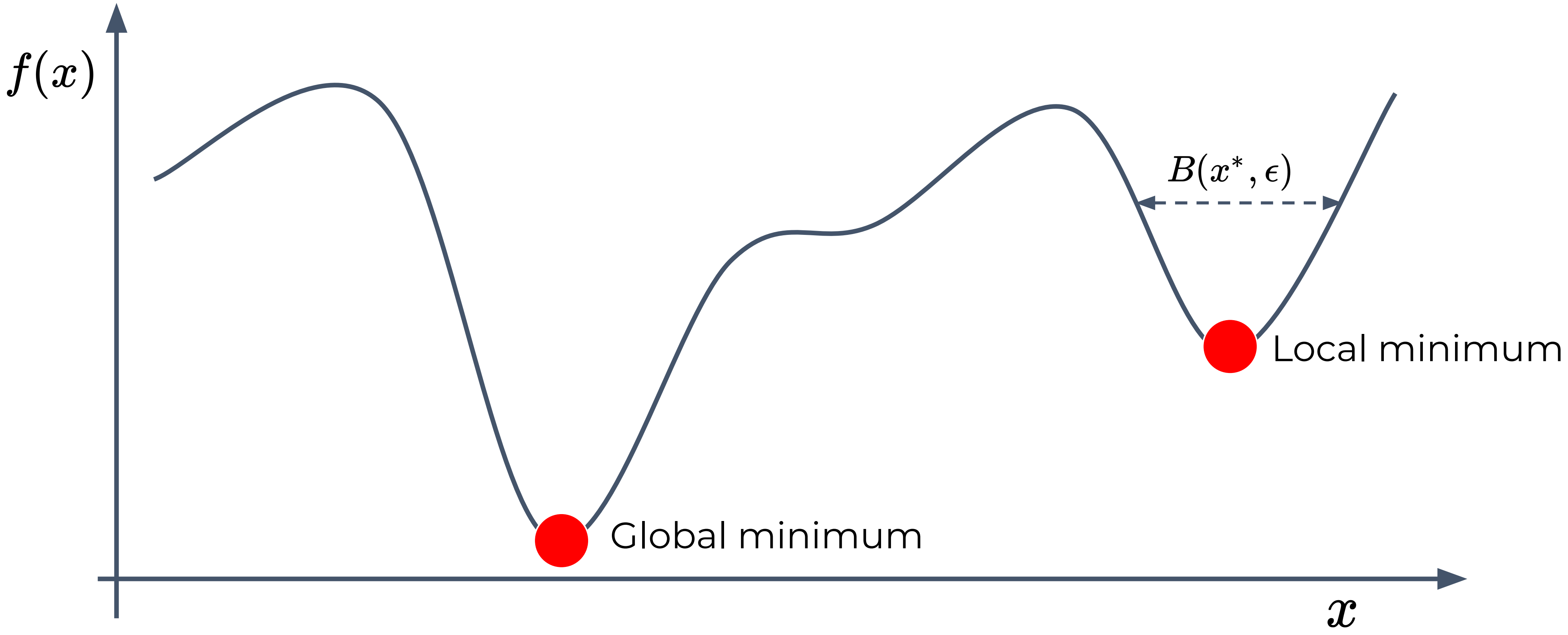
$$\exists \epsilon > 0, \forall x \in B(x^*, \epsilon), f(x^*) \leq f(x)$$



Example in 1D



Example



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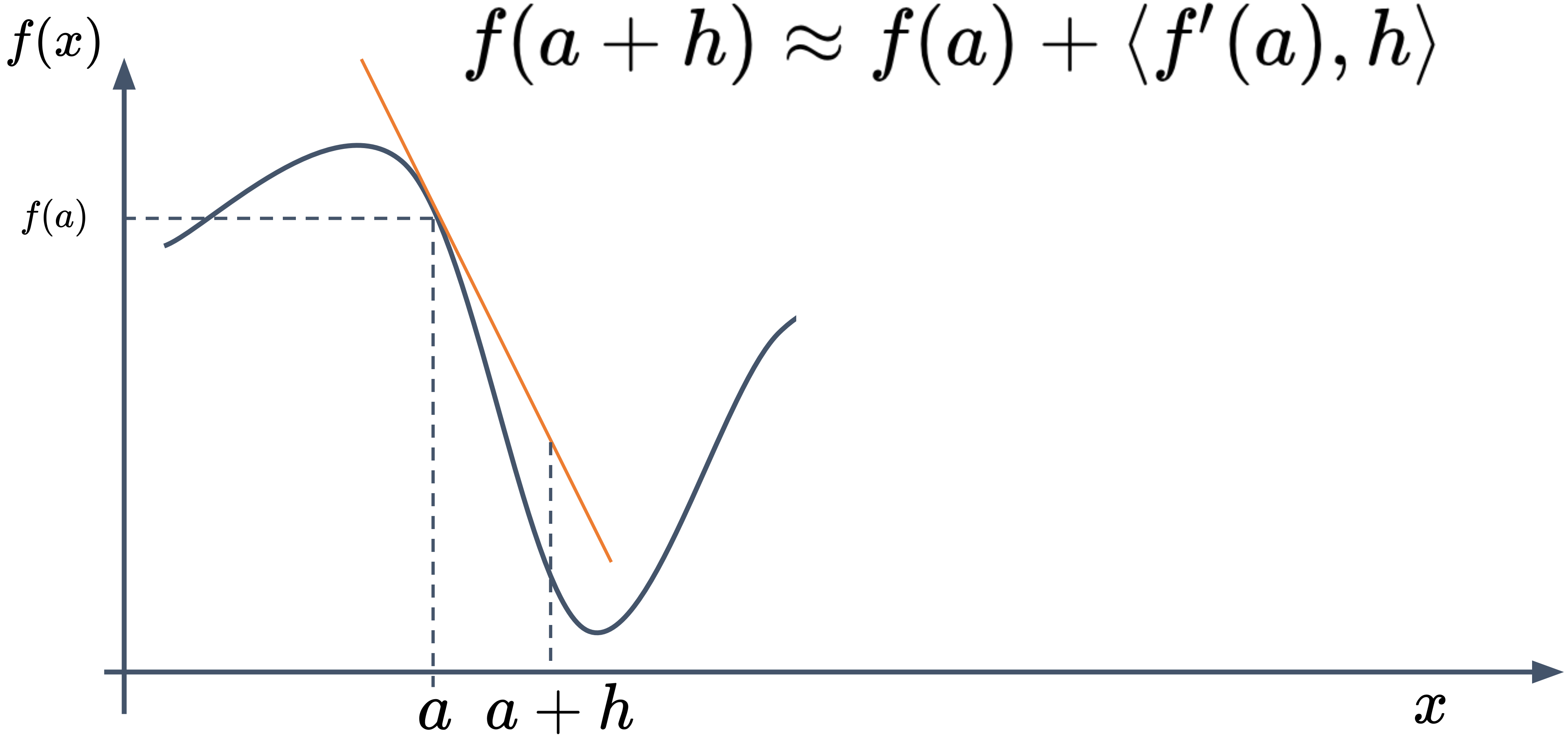
Linear approximation

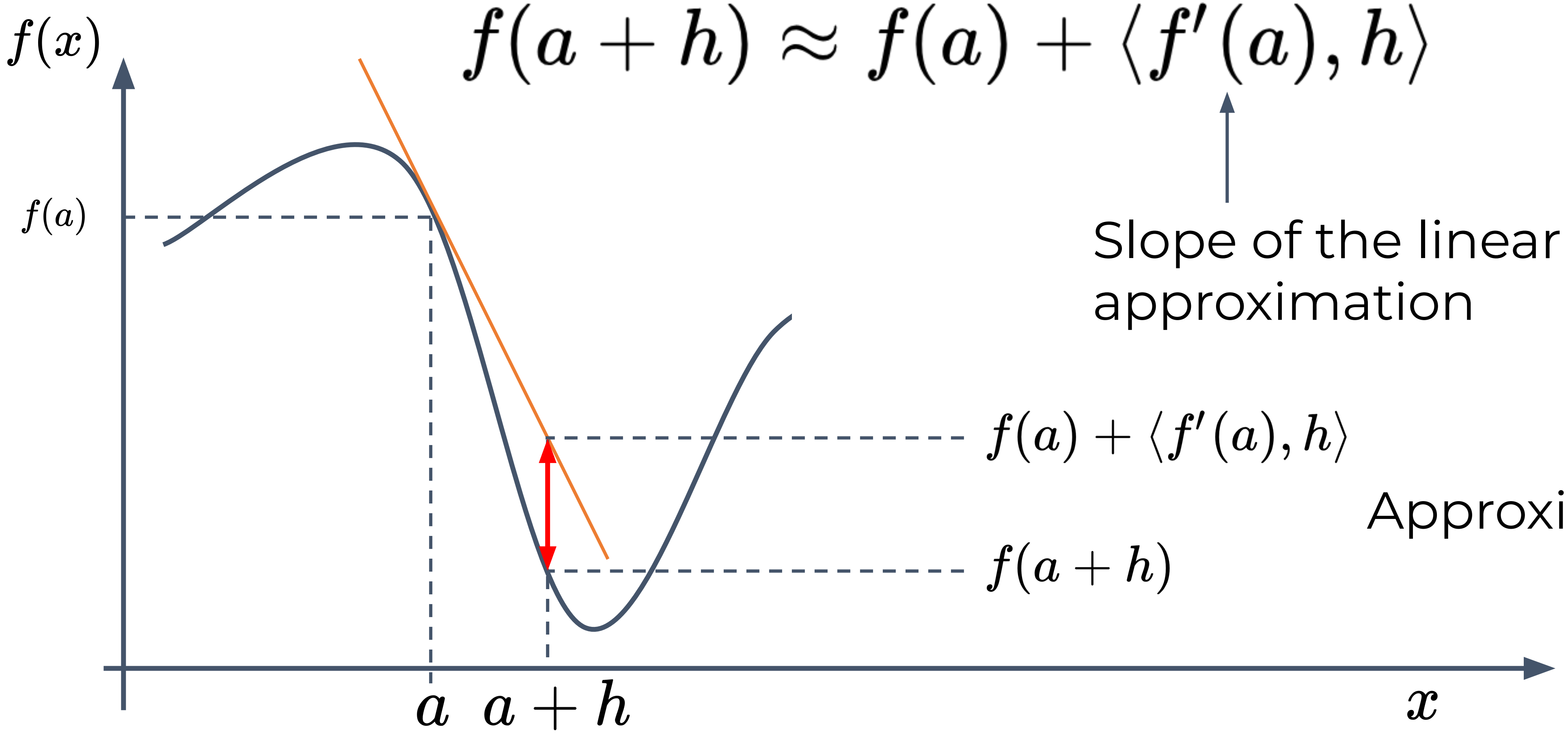
$$f(a+h) \approx f(a) + \langle f'(a), h \rangle$$



Linear approximation

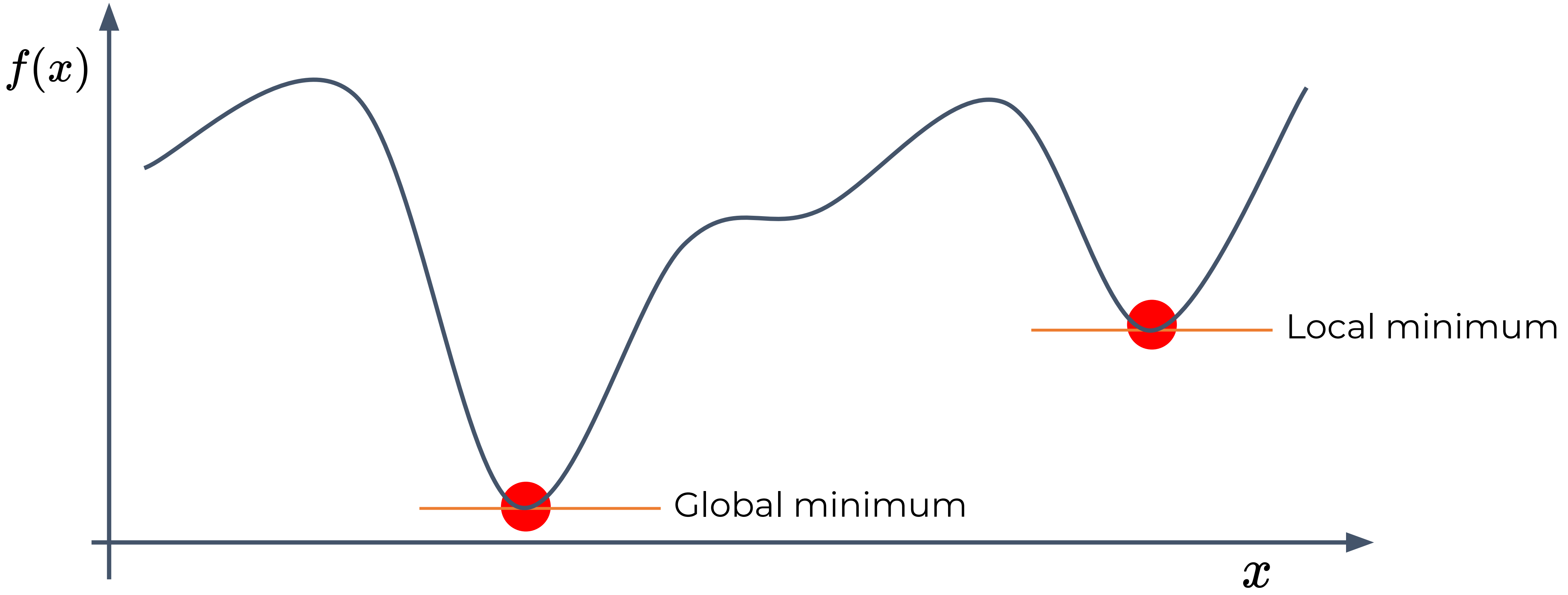
$$f(a+h) \approx f(a) + \langle f'(a), h \rangle$$

Slope of the linear approximation



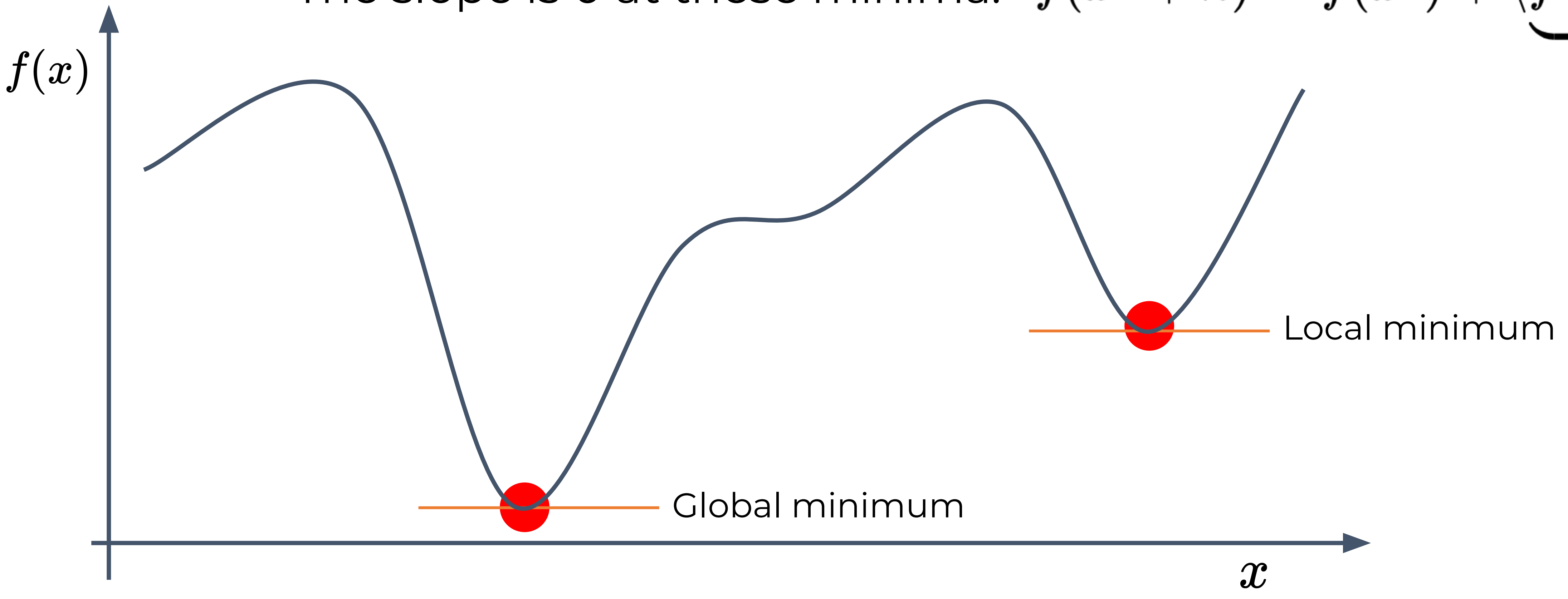
Approximation error

How to find extrema?



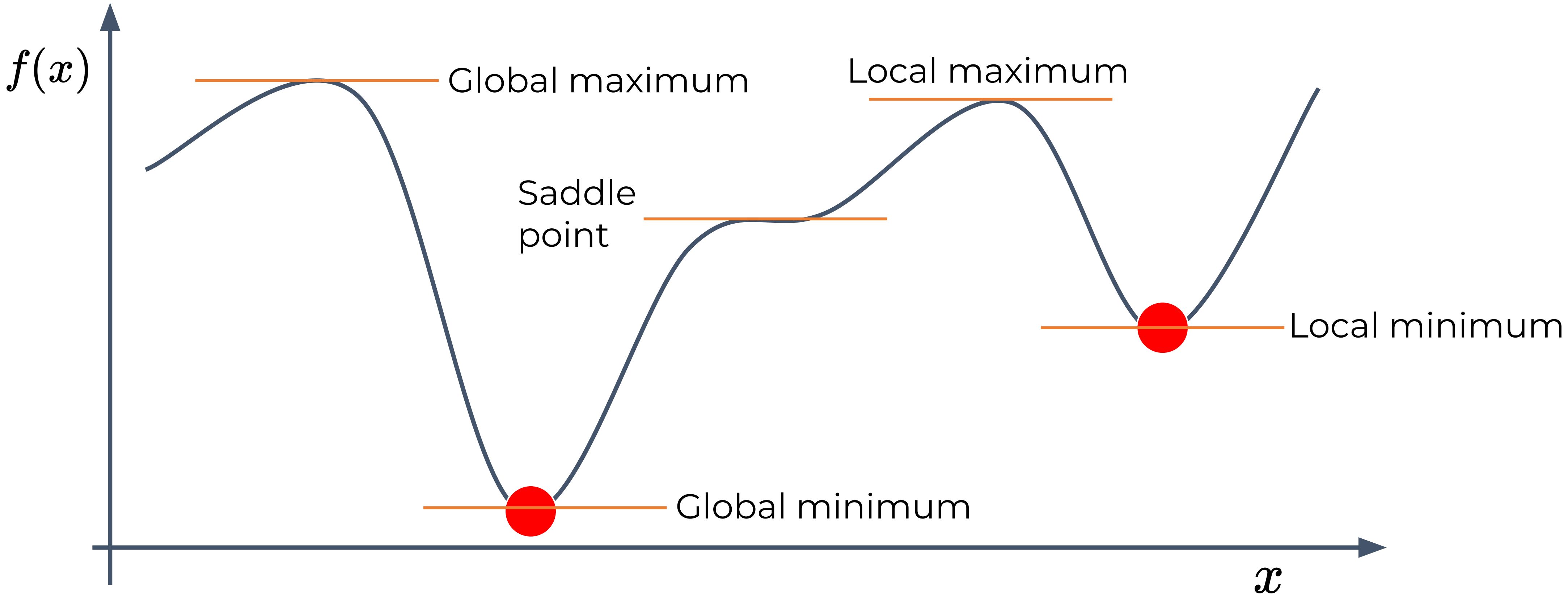
How to find extrema?

The slope is 0 at these minima: $f(x^* + h) \approx f(x^*) + \langle \underbrace{f'(x^*)}_{0}, h \rangle$



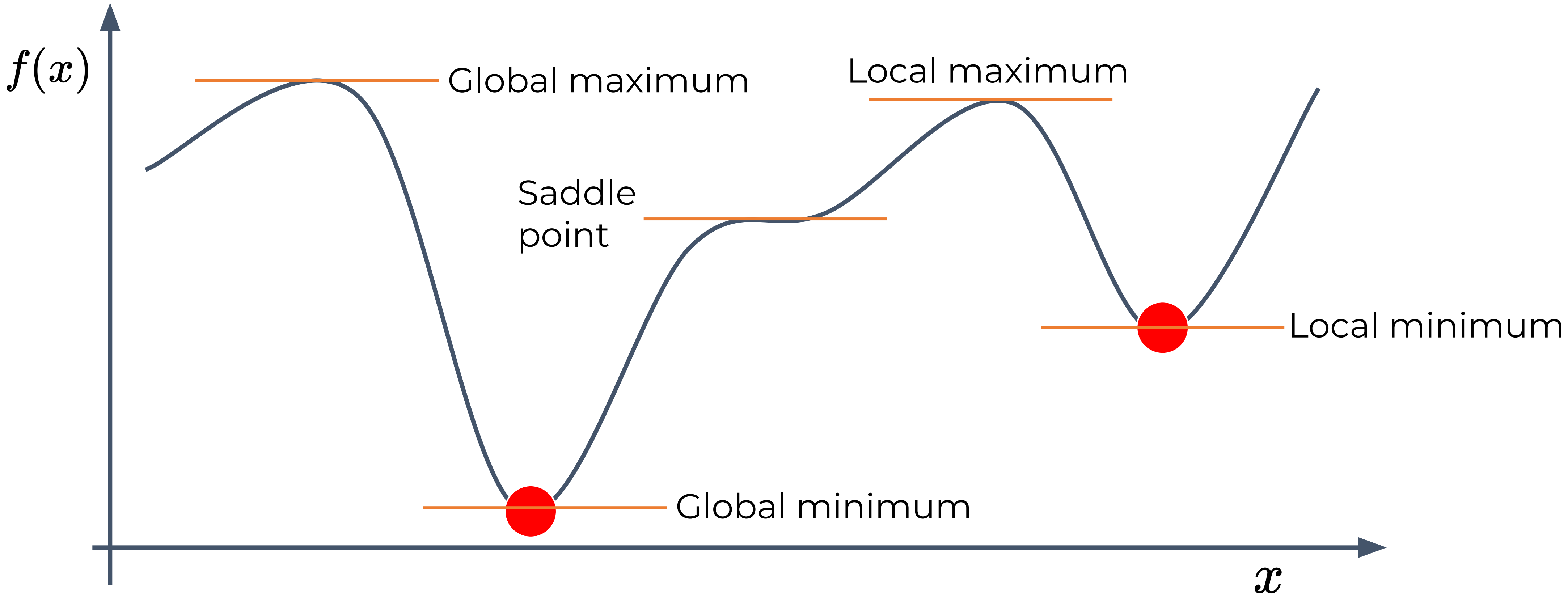
How to find extrema?

However, there are other points with a slope that equals 0.



Critical point classification

x^* is a critical point iif $f'(x^*) = 0$

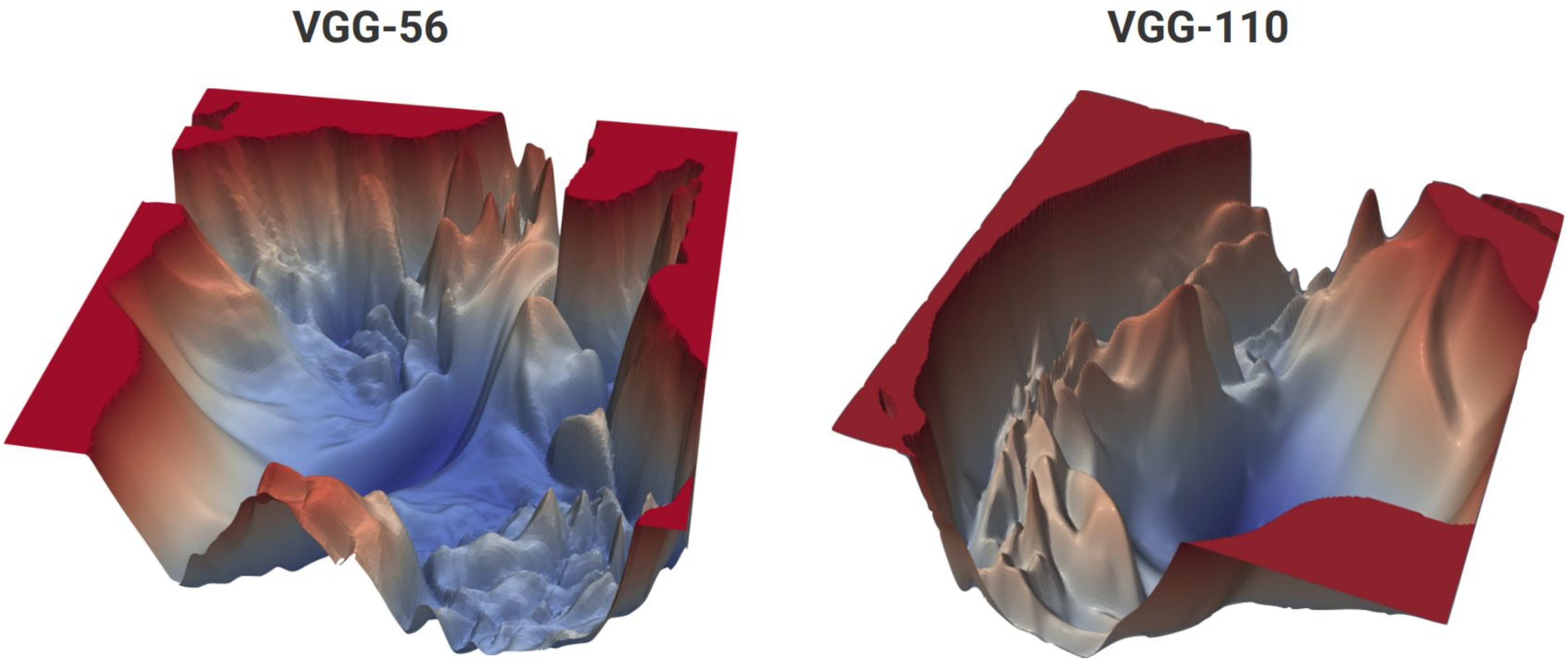


Fermat's theorem

If x^* is an extremum (local or global), then it is a critical point.

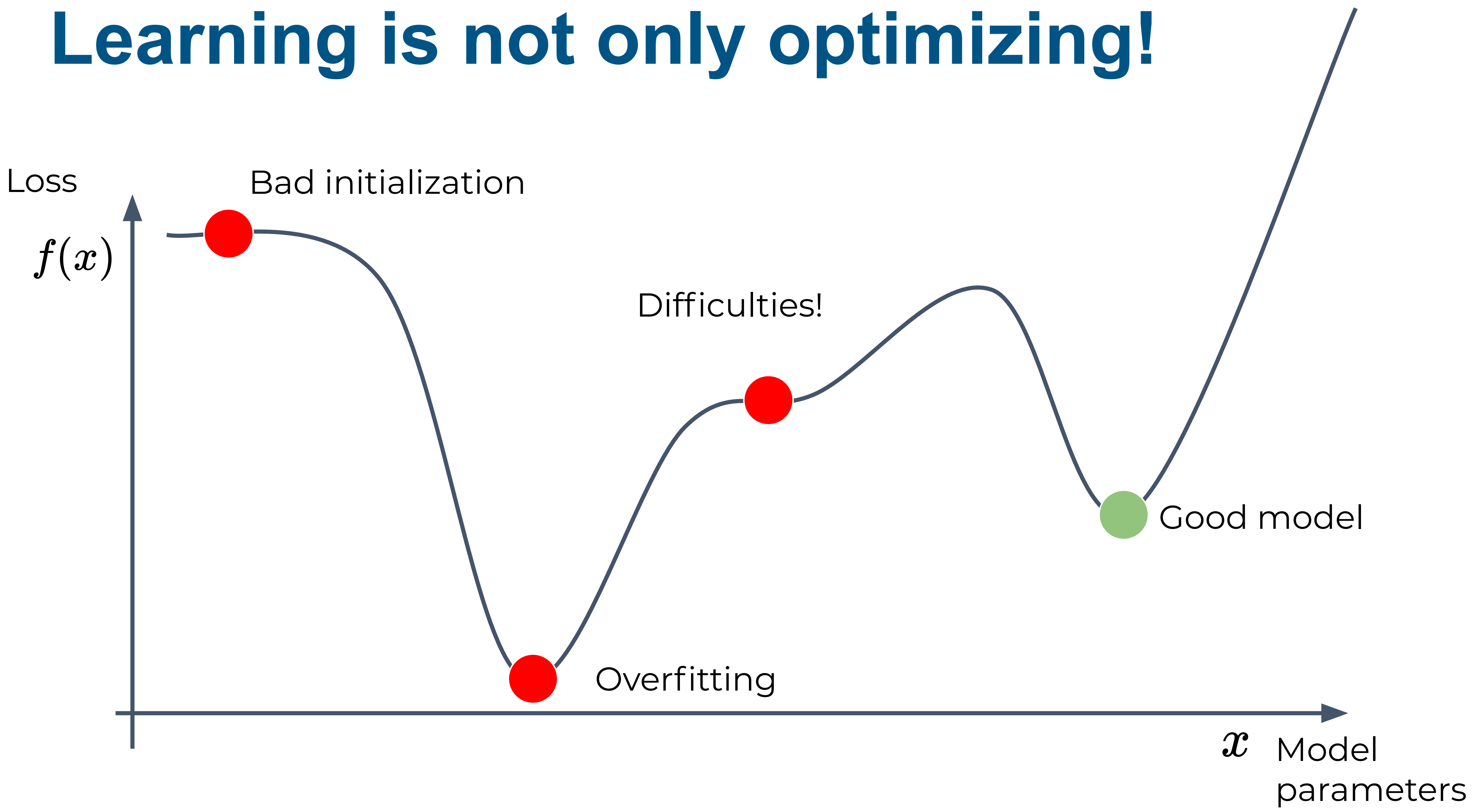
However, a critical point does not imply an extremum (e.g., a saddle point is not an extremum).

Parameter landscape for DL models



Li, Hao, et al. "Visualizing the loss landscape of neural nets." arXiv:1712.09913 (2017).

Learning is not only optimizing!



Critical point classification

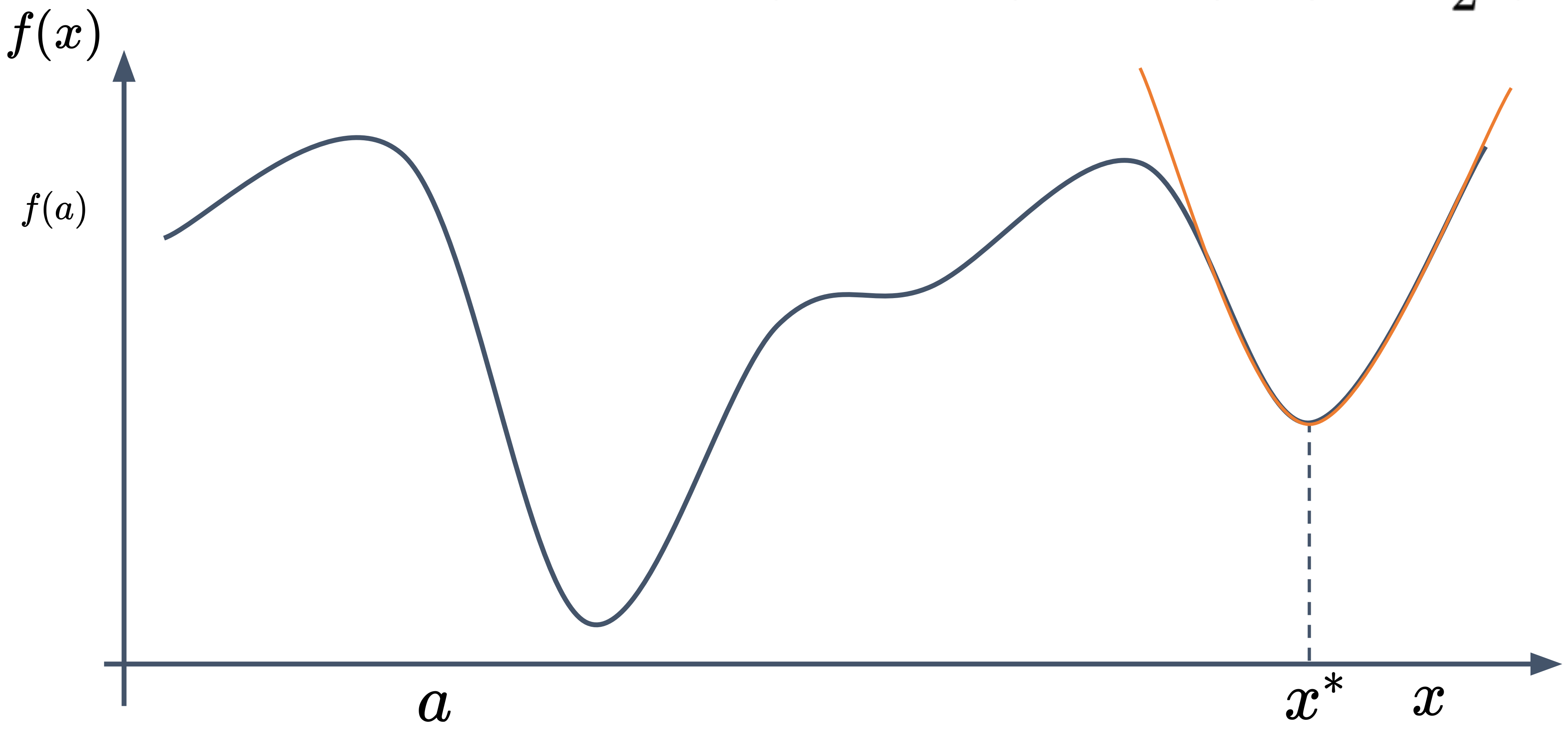
$$f(a+h) \approx f(a) + \langle f'(a), h \rangle + \frac{1}{2}\langle f''(a)h, h \rangle$$

Suppose that x^* is a minimum, then

$$f(x^* + h) \approx f(x^*) + \underbrace{\langle f'(x^*), h \rangle}_{0} + \underbrace{\frac{1}{2}\langle f''(x^*)h, h \rangle}_{q(h)}$$

Example

$$f(x^* + h) \approx f(x^*) + \frac{1}{2}\langle f''(x^*)h, h\rangle$$



Quadratic function in 2D

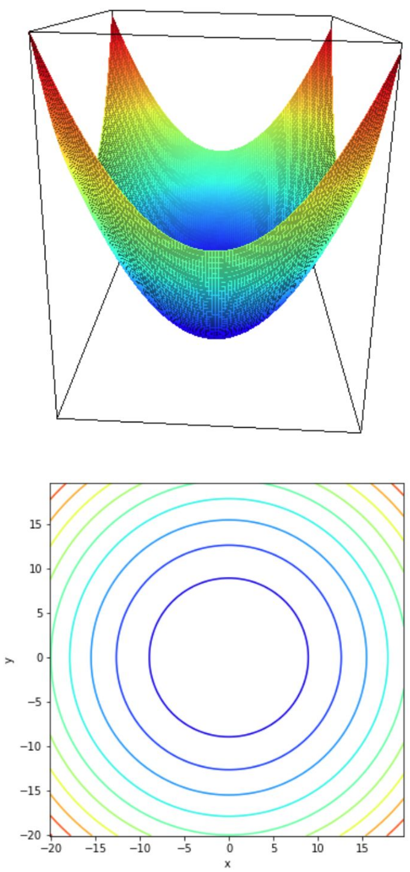
$$q(h) = \frac{1}{2}\langle f''(a)h, h\rangle$$

$$= \frac{1}{2}h^\top Hh = \frac{1}{2}\begin{bmatrix} h_1 & h_2 \end{bmatrix}\begin{bmatrix} \partial_{11}f(a) & \partial_{12}f(a) \\ \partial_{21}f(a) & \partial_{22}f(a) \end{bmatrix}\begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

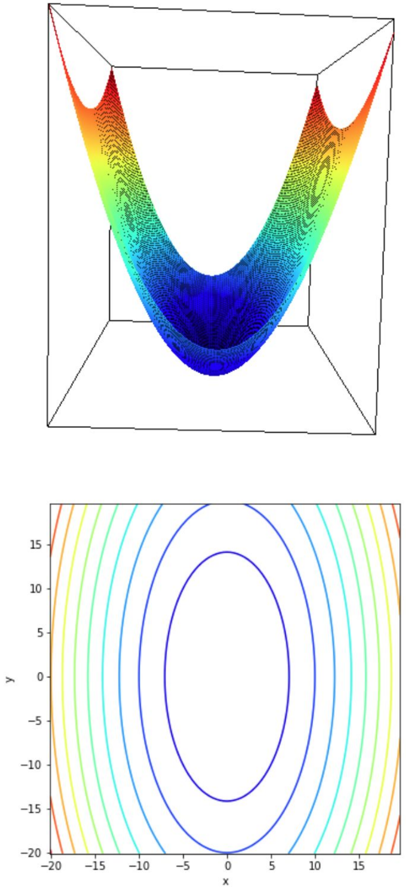
$$q'(h) = f''(a)h$$

$$\boxed{q''(h) = f''(a)}$$

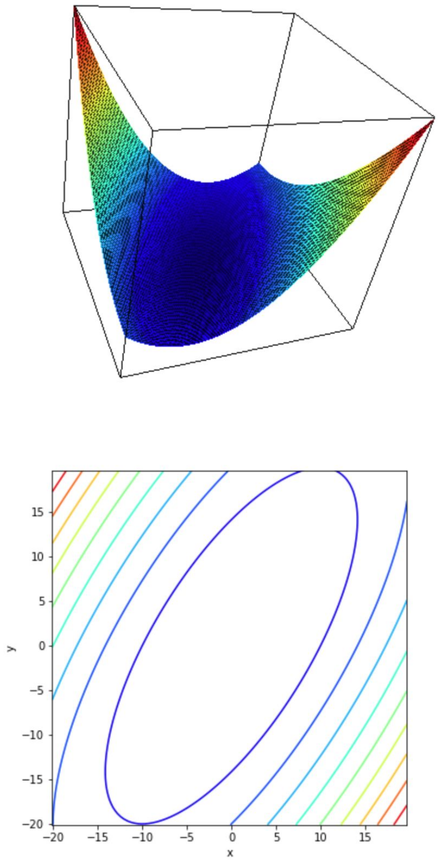
Positive definite in 2D



$$H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

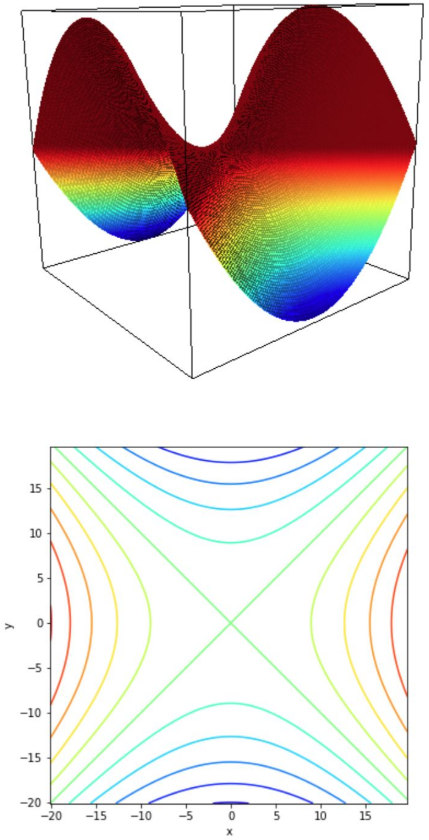


$$H = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$$

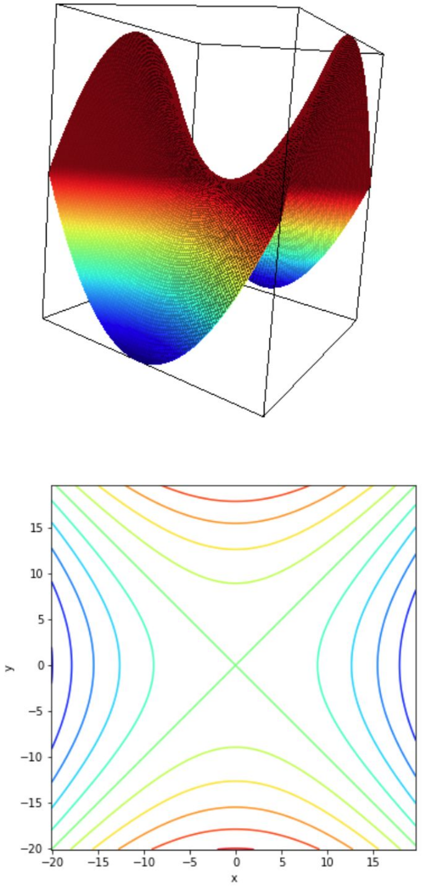


$$H = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}$$

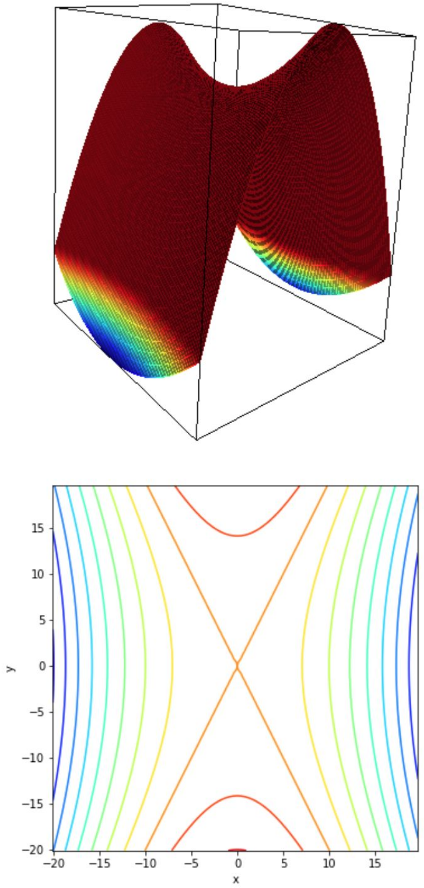
Saddle point in 2D



$$H = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$



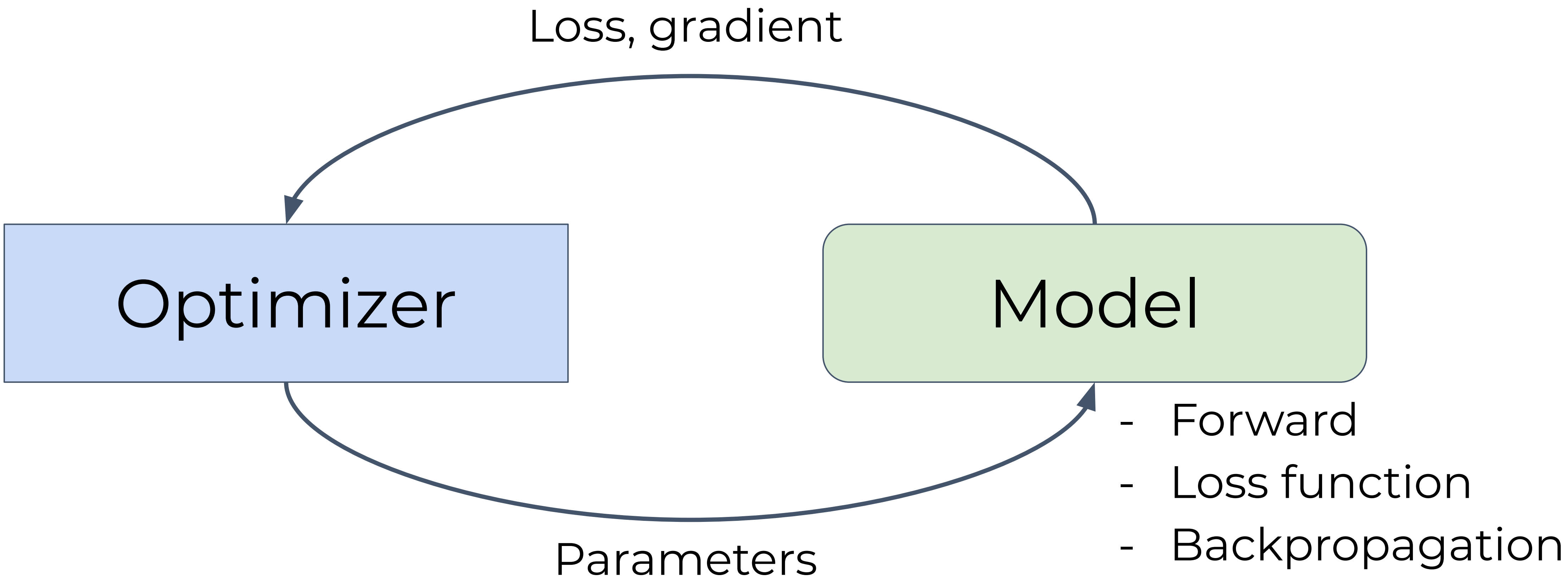
$$H = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$H = \begin{bmatrix} -4 & 0 \\ 0 & 1 \end{bmatrix}$$

Optimization algorithm

Iterative procedure



Why gradient is important for optimization?

$$f(a+h) - f(a) \approx \langle f'(a), h \rangle$$

h is a vector that gives the direction to go.

$$\begin{aligned} \min_{h, \|h\|=1} \langle f'(a), h \rangle &= \|f'(a)\| \|h\| \cos(\angle(f'(a), h)) \\ &= C \cos(\angle(f'(a), h)) \end{aligned}$$

The gradient indicates
the direction of the **steepest slope** at point a

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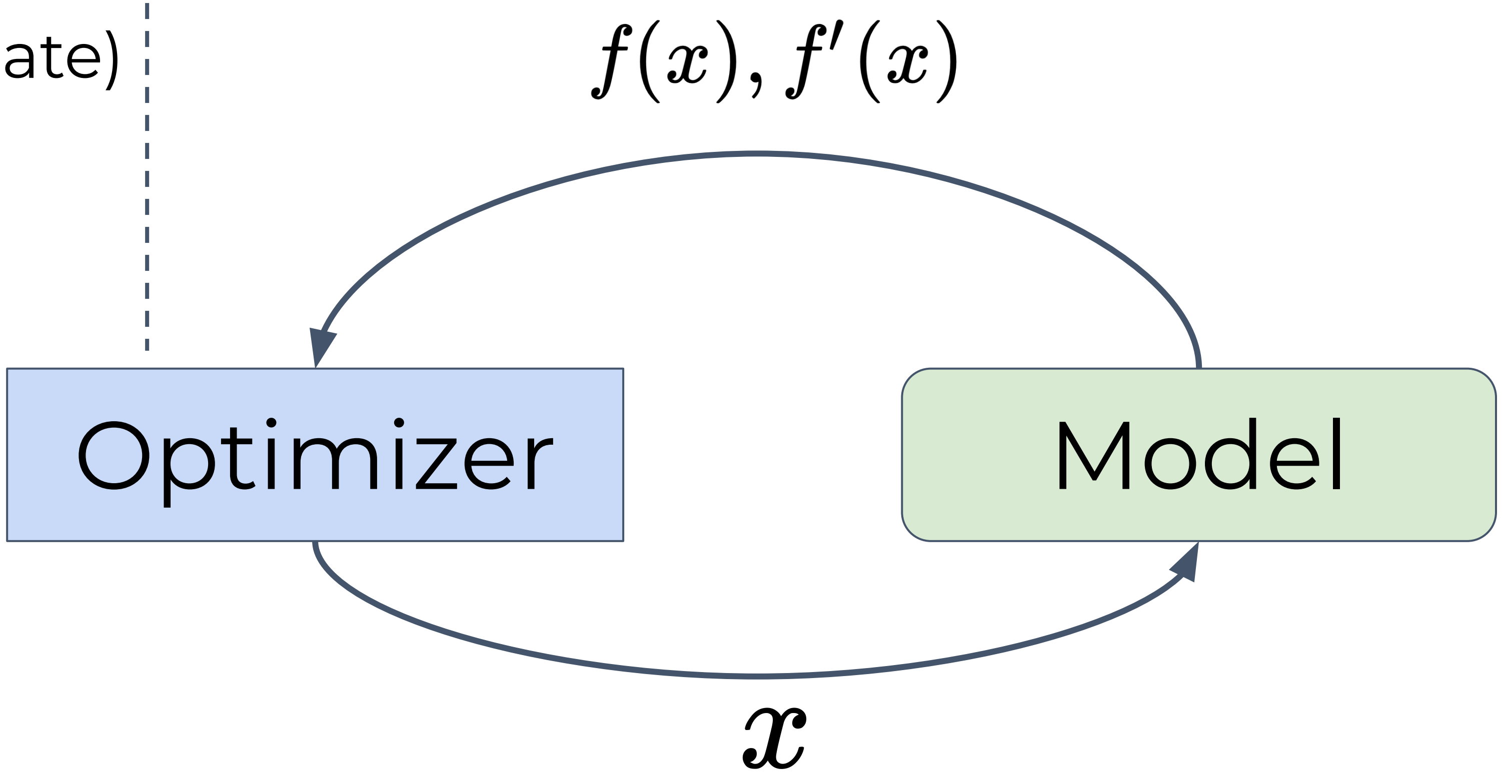
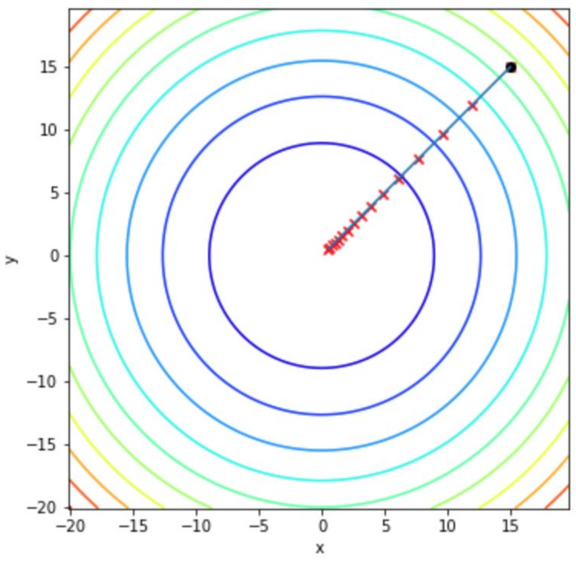
Steepest descent method (Gradient descent)

$$x_{t+1} \leftarrow x_t - \eta f'(x_t)$$

$\eta > 0$ (step-size, learning rate)

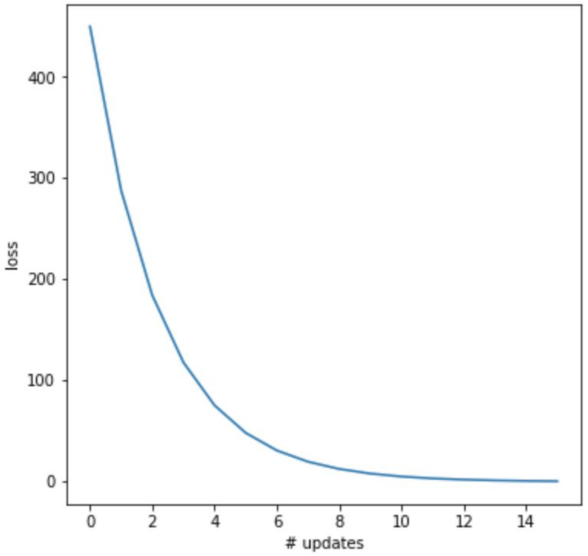


Gradient descent

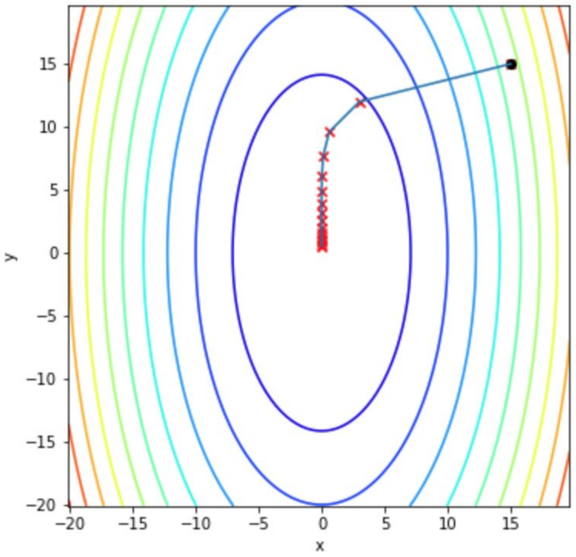


$$H = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\eta = 0.1$$

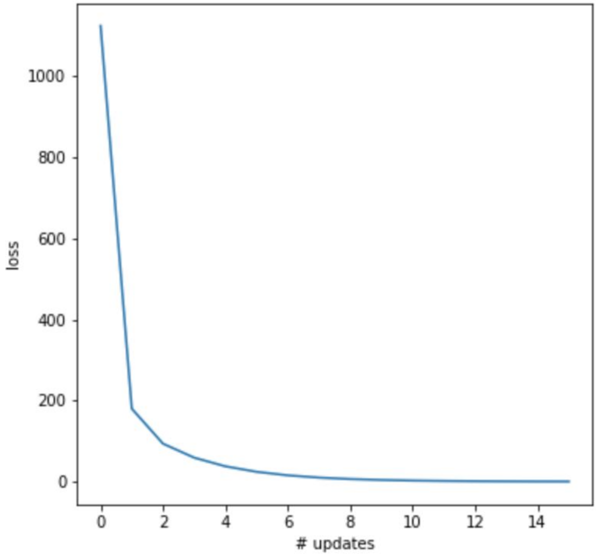


Gradient descent

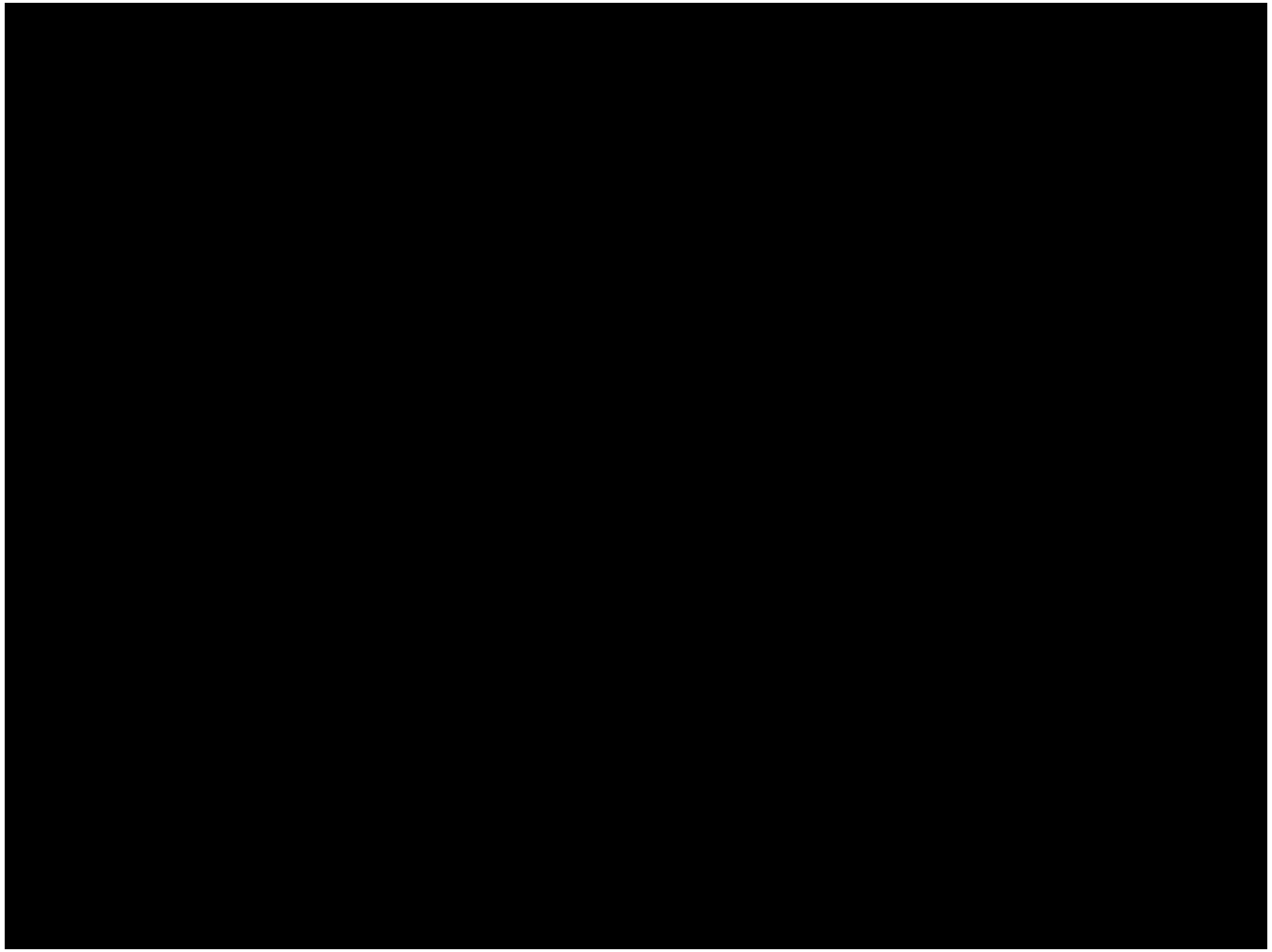


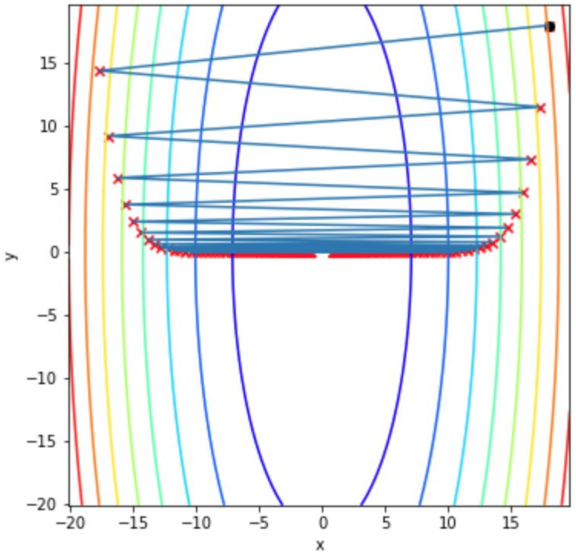
$$H = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\eta = 0.1$$



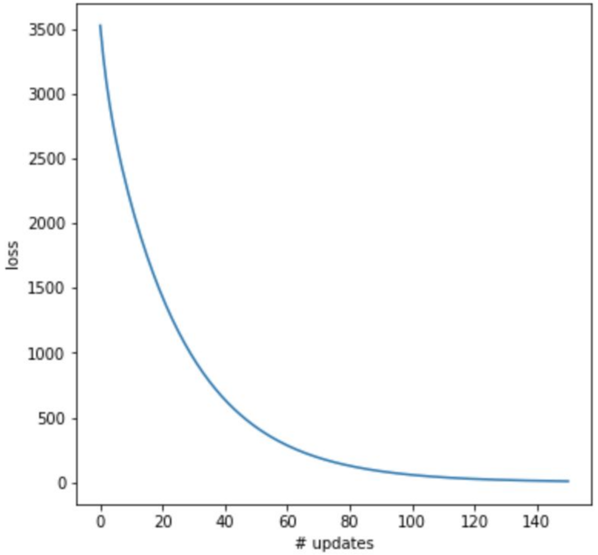
Gradient descent





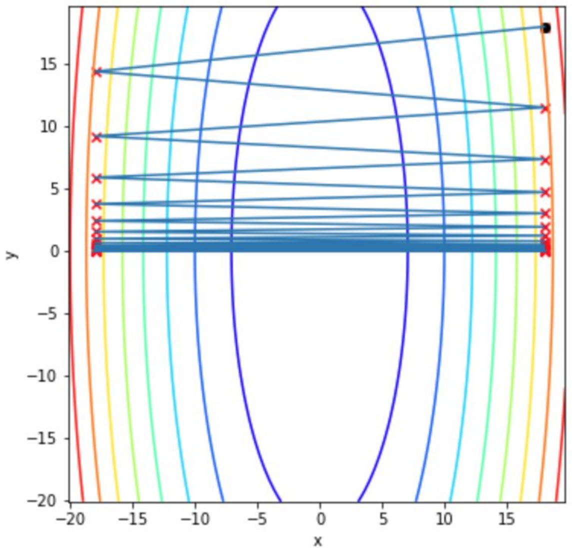
$$H = \begin{bmatrix} 9.9 & 0 \\ 0 & 1 \end{bmatrix}$$

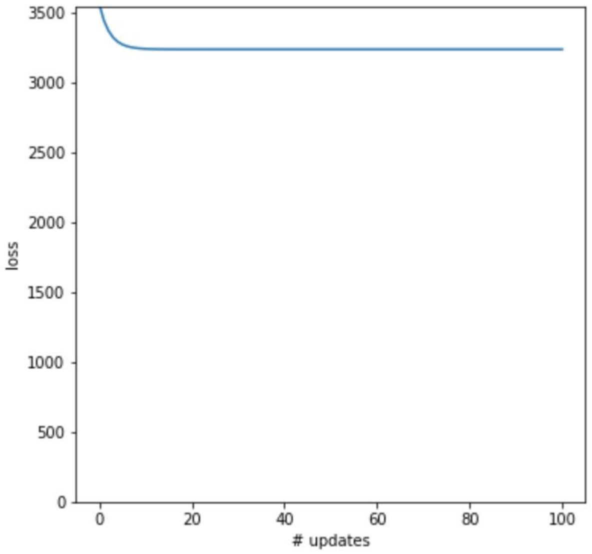
$$\eta = 0.1$$



Notice the rescaling of the axis.

Gradient descent





$$H = \begin{bmatrix} 10 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\eta = 0.1$$

Notice the rescaling of the axis.

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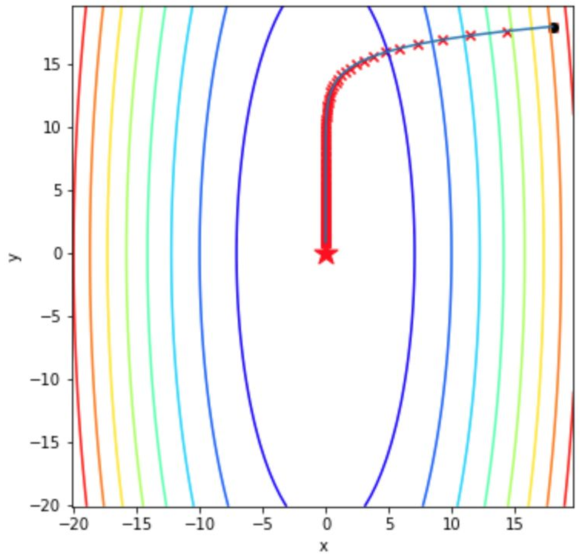
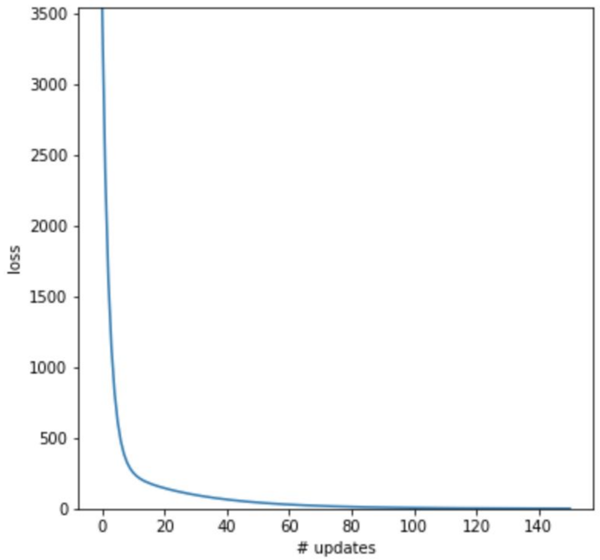
Gradient descent



$$H = \begin{bmatrix} 10 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\boxed{\eta = 0.01}$$



Notice the rescaling of the axis.

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Conditioning problem

How to quantify the problem? Condition number.

$$H = \begin{bmatrix} 10 & 0 \\ 0 & 1 \end{bmatrix} \qquad \kappa(H) = \frac{|10|}{|1|}$$

We want to have a condition number close to 1.

Problem of physical units

What are the physical units of this equation?

$$x_{t+1} \leftarrow x_t - \eta f'(x_t)$$

2D example:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \eta \begin{bmatrix} \partial_1 f(x) \\ \partial_2 f(x) \end{bmatrix}$$

x_1 : [km] x_2 : [mm] η : [?]

$\partial_1 f(x)$: [J/km] $\partial_2 f(x)$: [J/mm]

Problem of physical units

What are the physical units of this equation?

$$x_{t+1} \leftarrow x_t - \eta M_t f'(x_t)$$

2D example:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \eta \begin{bmatrix} M_{11} & 0 \\ 0 & M_{22} \end{bmatrix} \begin{bmatrix} \partial_1 f(x) \\ \partial_2 f(x) \end{bmatrix}$$

x_1 : [km] x_2 : [mm] M_{11} : [km²/J]

$\partial_1 f(x)$: [J/km] $\partial_2 f(x)$: [J/mm] M_{22} : [mm²/J]

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Preconditioning

General update equation for gradient descent.

$$x_{t+1} \leftarrow x_t - \eta M_t f'(x_t)$$

M : preconditioning matrix

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \eta \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \partial_1 f(x) \\ \partial_2 f(x) \end{bmatrix}$$

Preconditioning

General update equation for gradient descent.

$$x_{t+1} \leftarrow x_t - \eta M_t f'(x_t)$$

The size of M_t is (number of parameters)^2!

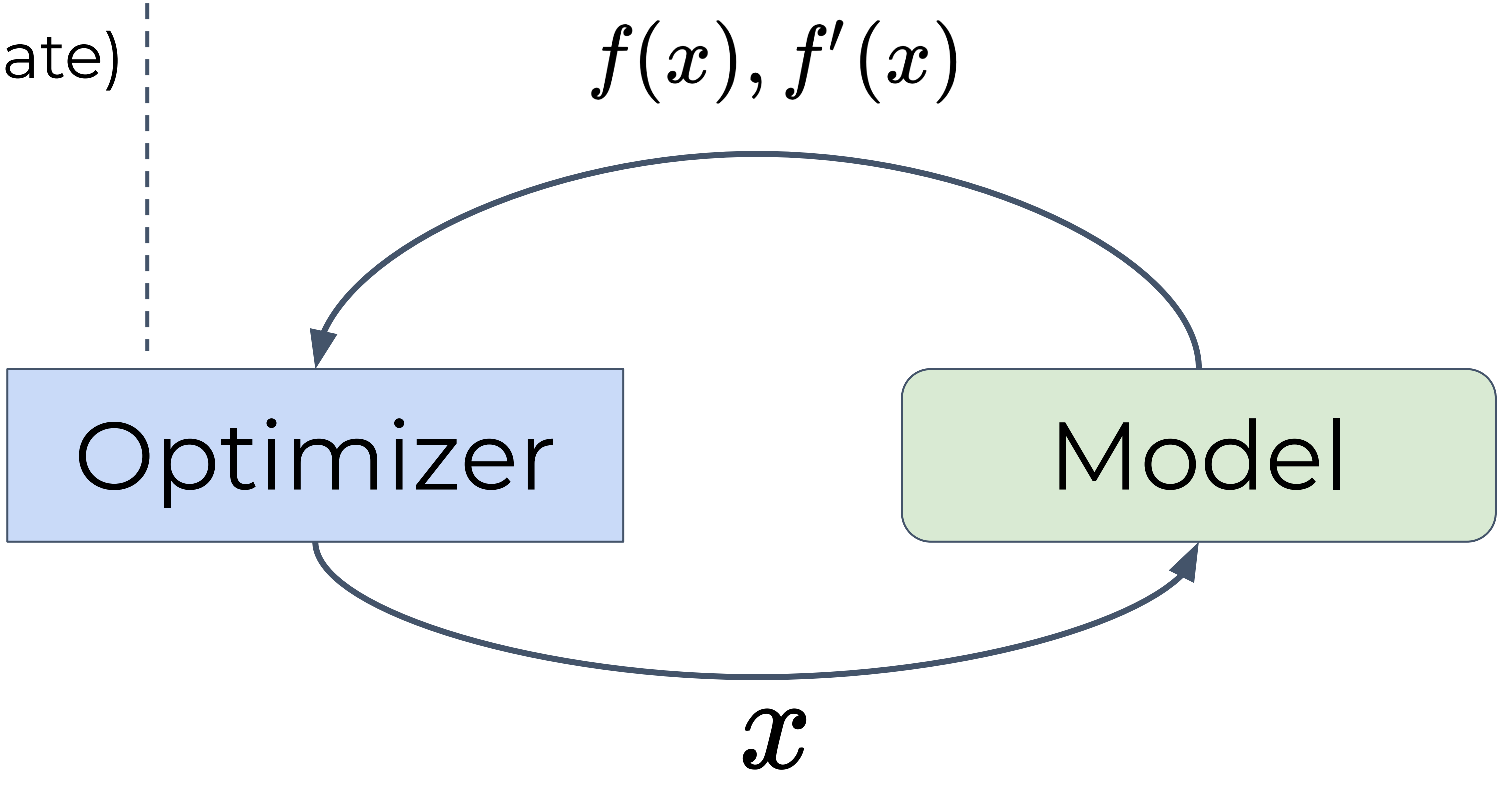
M : preconditio

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \eta \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} \partial_1 f(x) \\ \partial_2 f(x) \end{bmatrix}$$

Preconditioned gradient descent

$$x_{t+1} \leftarrow x_t - \eta M_t f'(x_t)$$

$\eta > 0$ (step-size, learning rate)



RMSProp

Component-wise preconditioning

$$v_t = \beta v_{t-1} + (1-\beta) f'(x_t)^2$$

Preconditioning term

$$x_{t+1} = x_t + \frac{1}{\sqrt{v_t + \epsilon}} f'(x_t)$$

Update rule

Momentum

- Potential energy $U(x) = mgh(x)$

$$F = ma = -U'(x) = -mgh'(x)$$

Source:Sam Poullain, Unsplash

Initial conditions: x_0, v_0

Physics	Optimization
$a_t \leftarrow -gh'(x_t)$	$a_t \leftarrow -\eta f'(x_t)$
$v_{t+1} \leftarrow \mu v_t + a_t \Delta t$	$v_{t+1} \leftarrow \mu v_t + a_t$
$x_{t+1} \leftarrow x_t + v_{t+1} \Delta t$	$x_{t+1} \leftarrow x_t + v_{t+1}$

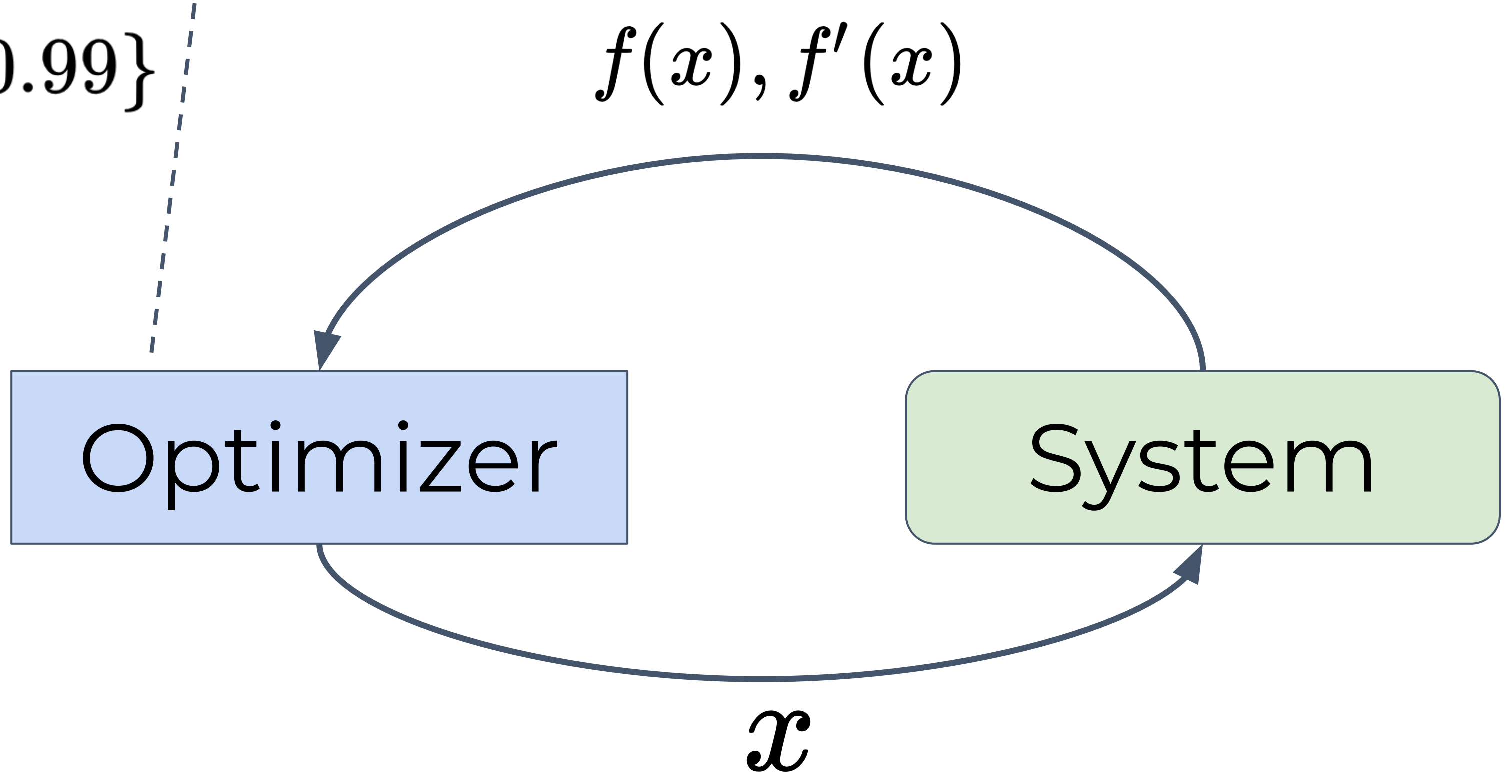
μ : friction

Gradient descent with momentum

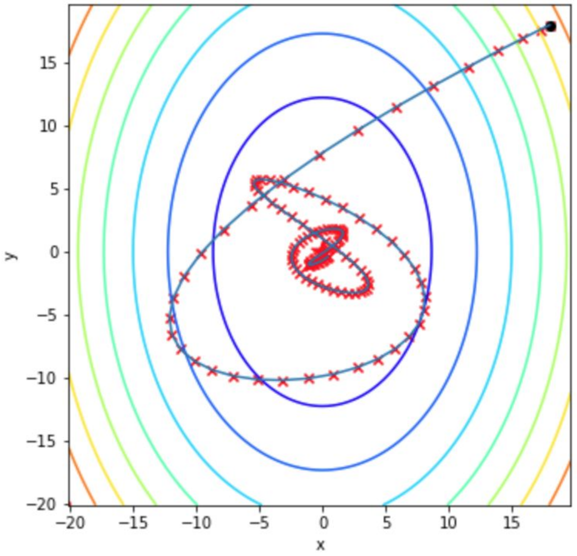
$$v \leftarrow \mu v - \eta f'(x)$$

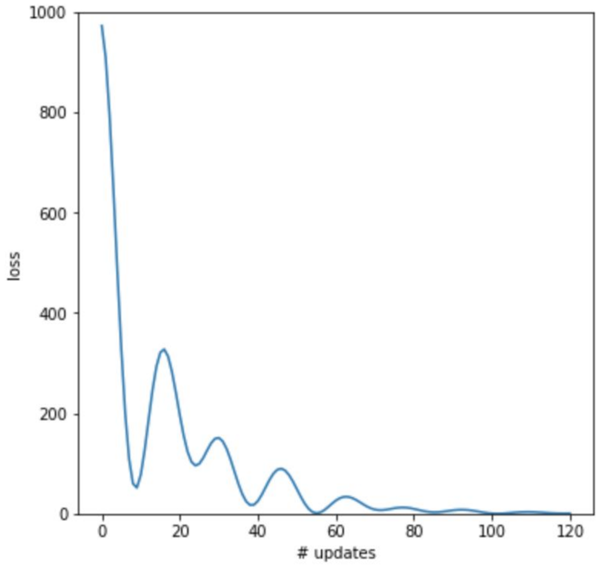
$$x \leftarrow x + v$$

$\eta > 0 \quad \mu \in \{0.5, 0.9, 0.95, 0.99\}$



Momentum



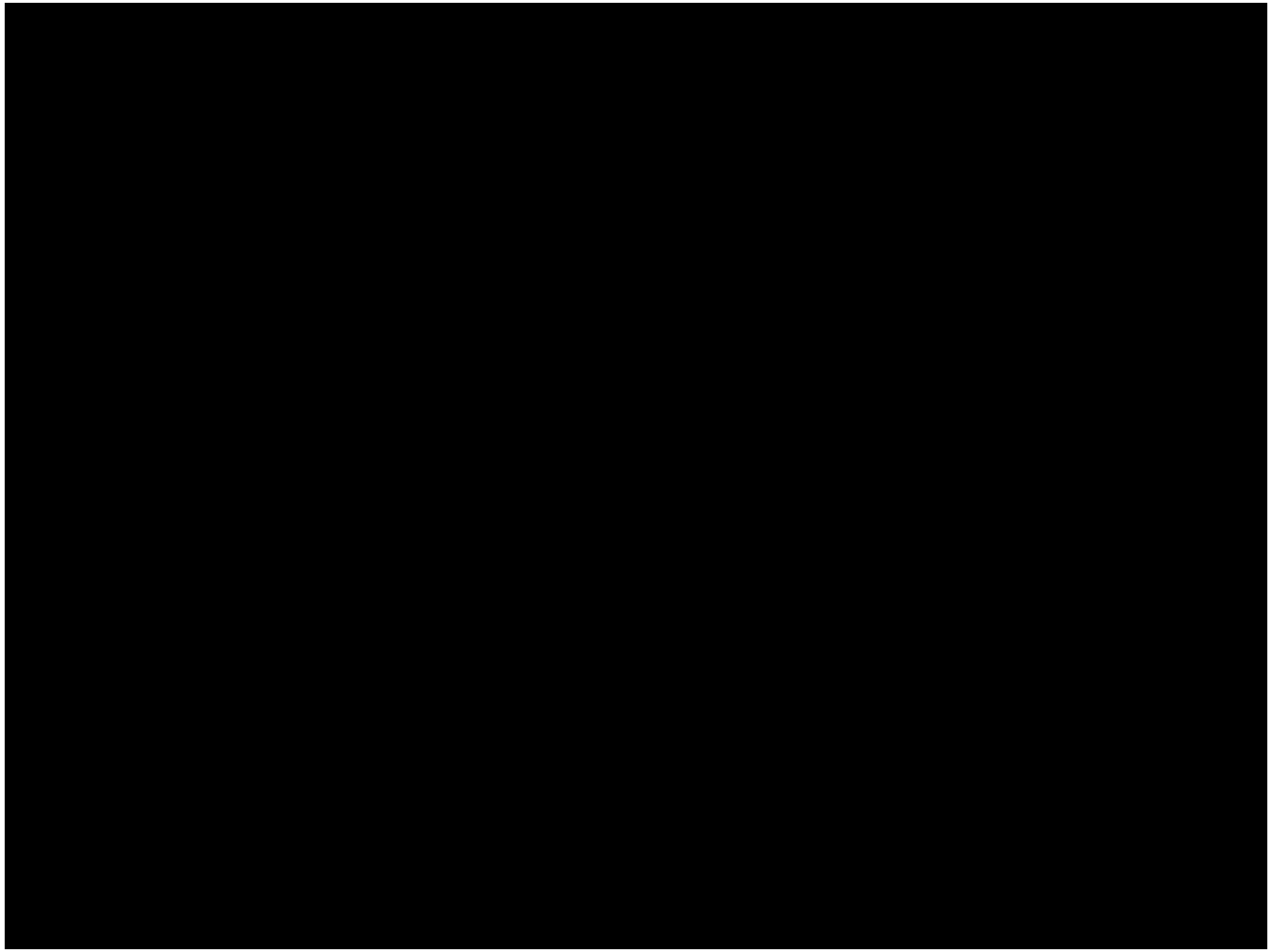


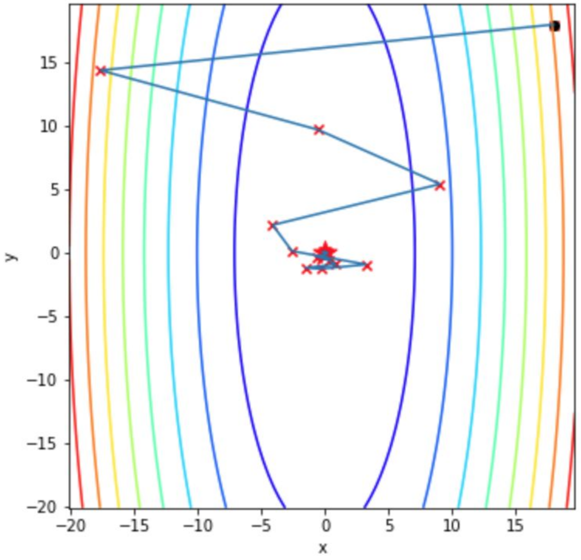
$$H = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

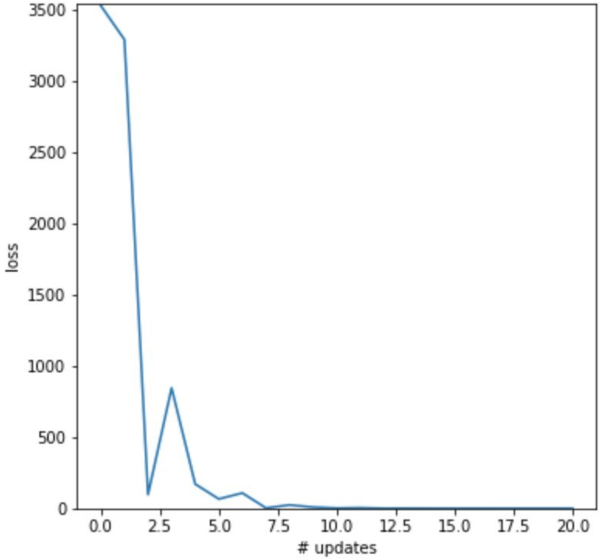
$$\eta = 0.01$$

$$\mu = 0.95$$

Momentum







$$H = \begin{bmatrix} 9.9 & 0 \\ 0 & 1 \end{bmatrix}$$

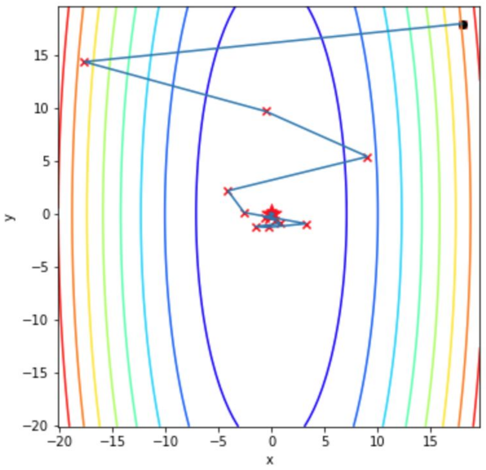
$$\eta = 0.1$$

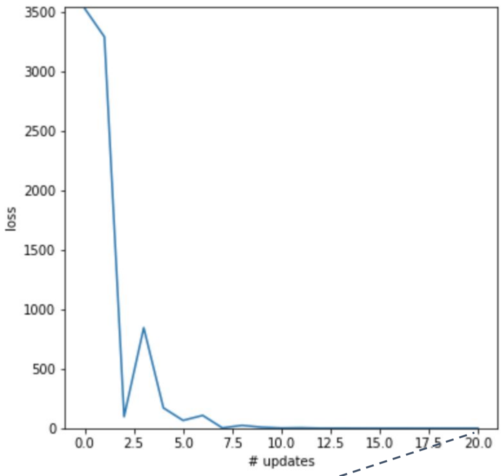
$$\mu = 0.5$$

Comparison

$$H = \begin{bmatrix} 9.9 & 0 \\ 0 & 1 \end{bmatrix}$$

With Momentum

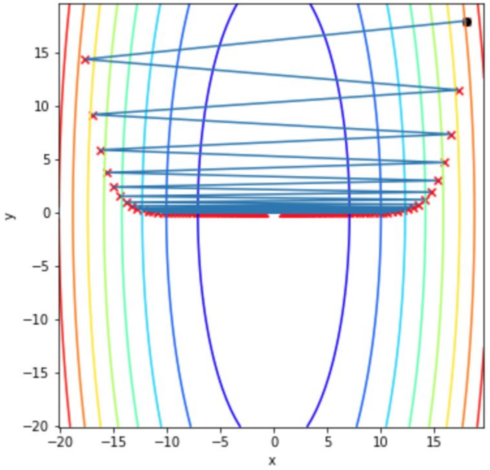


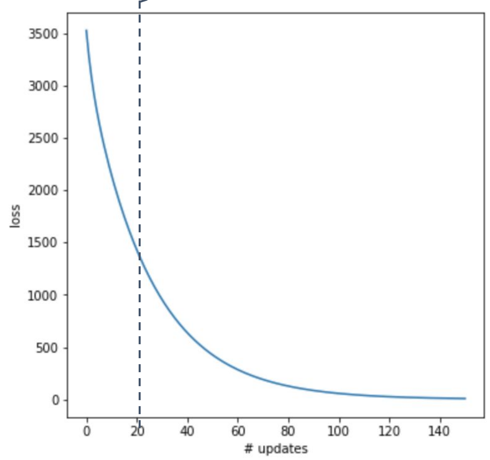


$$\eta = 0.1$$

$$\mu = 0.5$$

Without Momentum

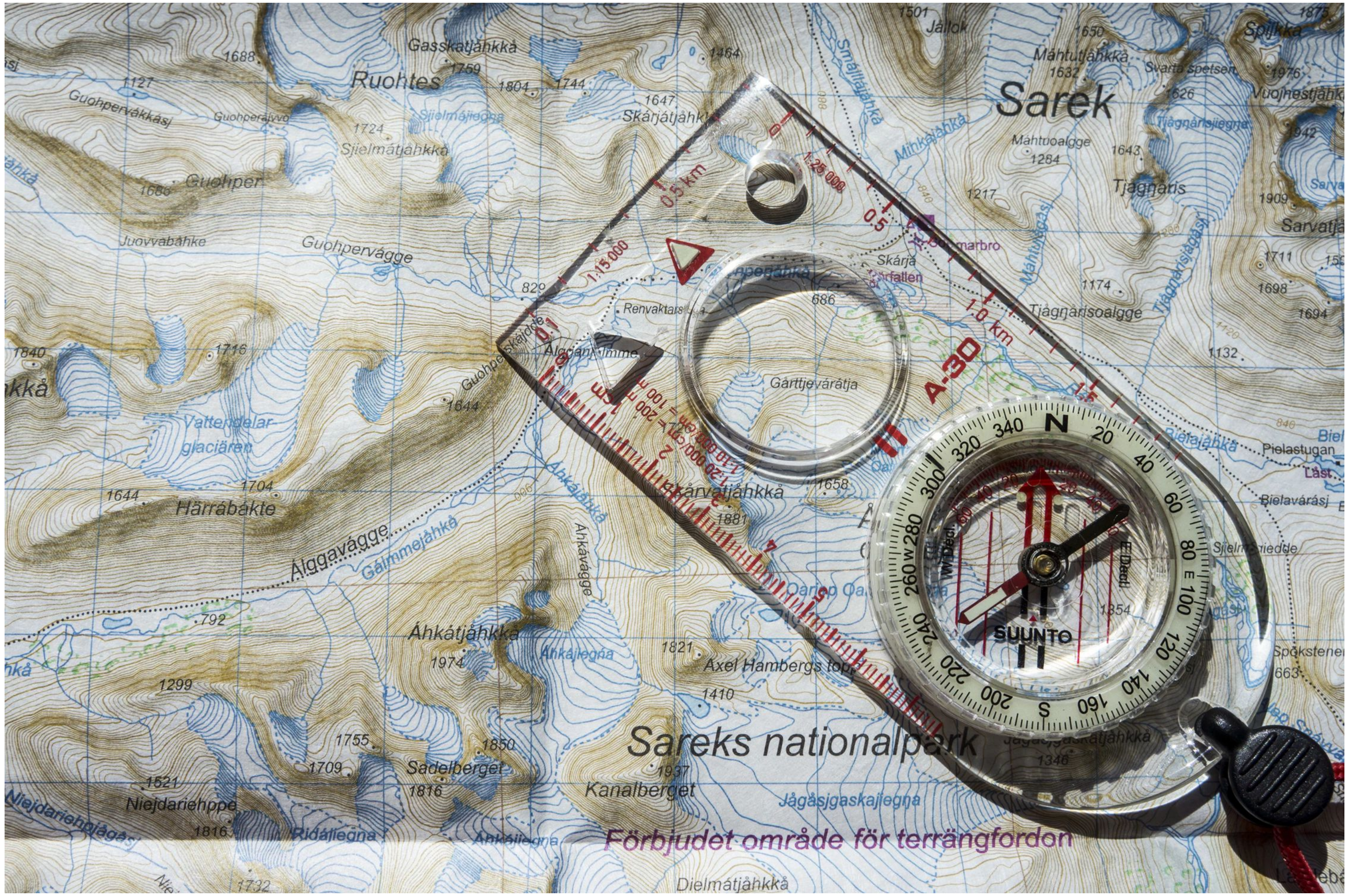




$$\eta = 0.1$$

A family of algorithms

- Adagrad
- Adadelta
- AdaMax
- RMSProp
- **Adam**
- AMSGrad
- ...



Source: Hendrik Morkel, Unsplash

Adaptive moment estimation (Adam)
RMSProp with momentum

Component-wise preconditioning

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) f'(x_t)$$ Momentum term

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) f'(x_t)^2$$ Preconditioning term

$$x_{t+1} = x_t + \frac{1}{\sqrt{v_t} + \epsilon} m_t$$ Update rule

This is a simplified version without the bias correction terms!

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Stochastic optimization

Stochastic gradient descent

Risk

$$L(\theta) = \mathbb{E}_{z \sim \mathcal{D}} \left[l(\theta; z) \right]$$

Stochastic gradient descent

Risk

Empirical risk

$$L(\theta) = \mathbb{E}_{z\sim\mathcal{D}}\left[l(\theta; z)\right] \xrightarrow{\text{Approximation 1}} \hat{L}(\theta) = \frac{1}{N}\sum_{i=1}^{N} l(\theta; z_i)$$

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Stochastic gradient descent

Risk

$$L(\theta) = \mathbb{E}_{z\sim\mathcal{D}}\left[l(\theta; z)\right]$$

Empirical risk

$$\hat{L}(\theta) = \frac{1}{N}\sum_{i=1}^{N} l(\theta; z_i)$$

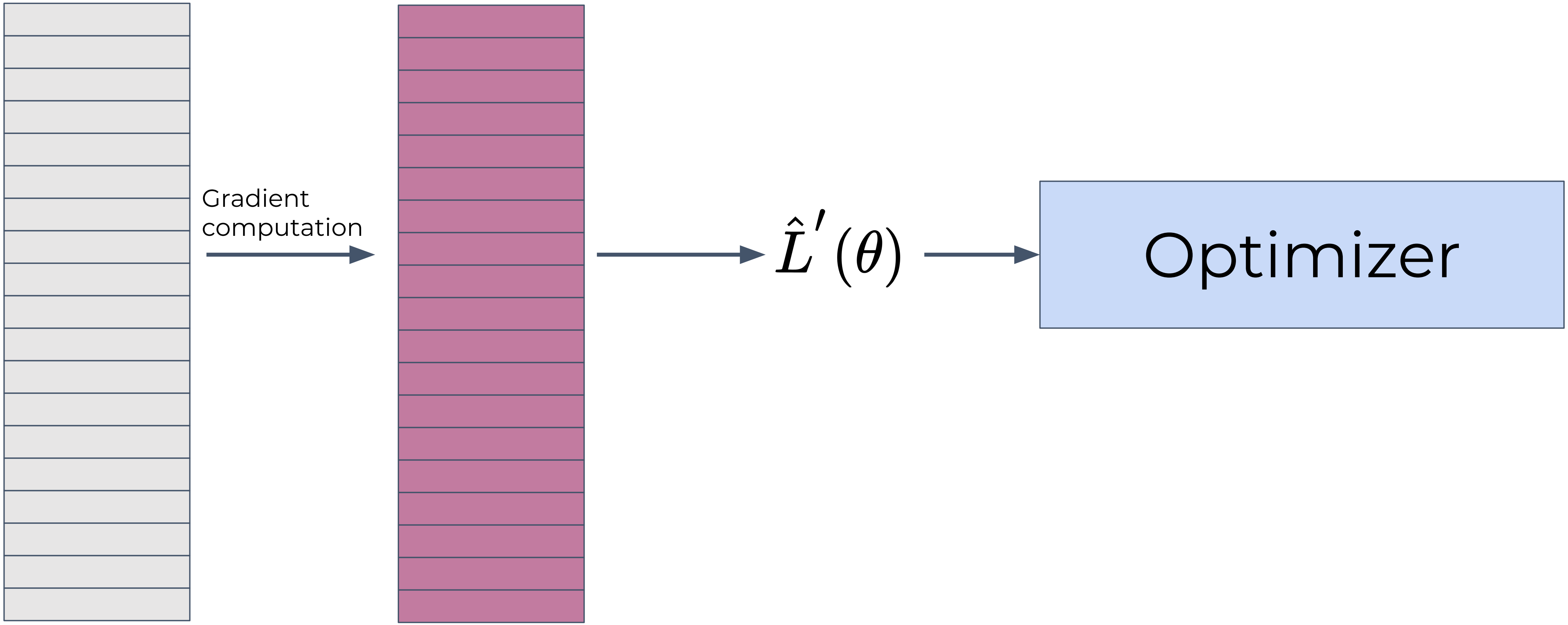
Approximation 1

Approximation 2

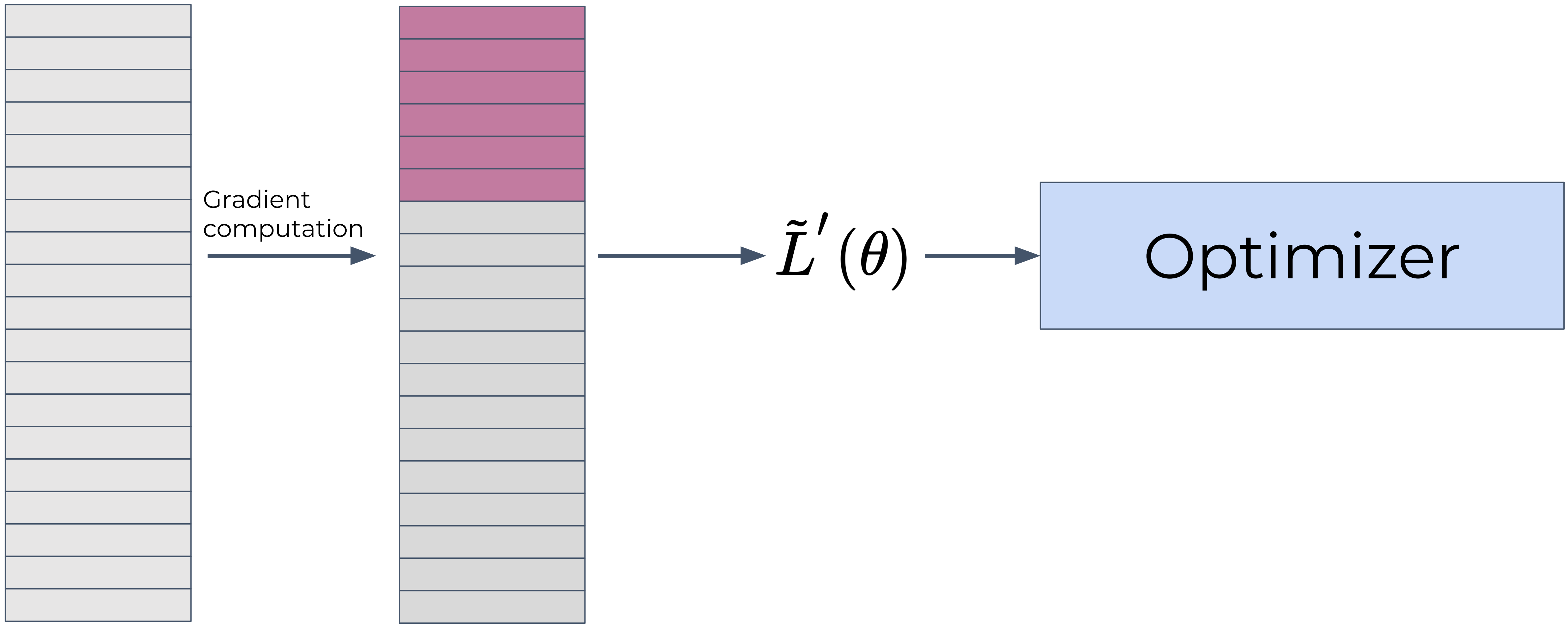
$$\tilde{L}(\theta) = \frac{1}{K}\sum_{i=1}^{K} l(\theta; z_{\sigma(i)})$$

K<<N : Number of examples (Mini-batch)

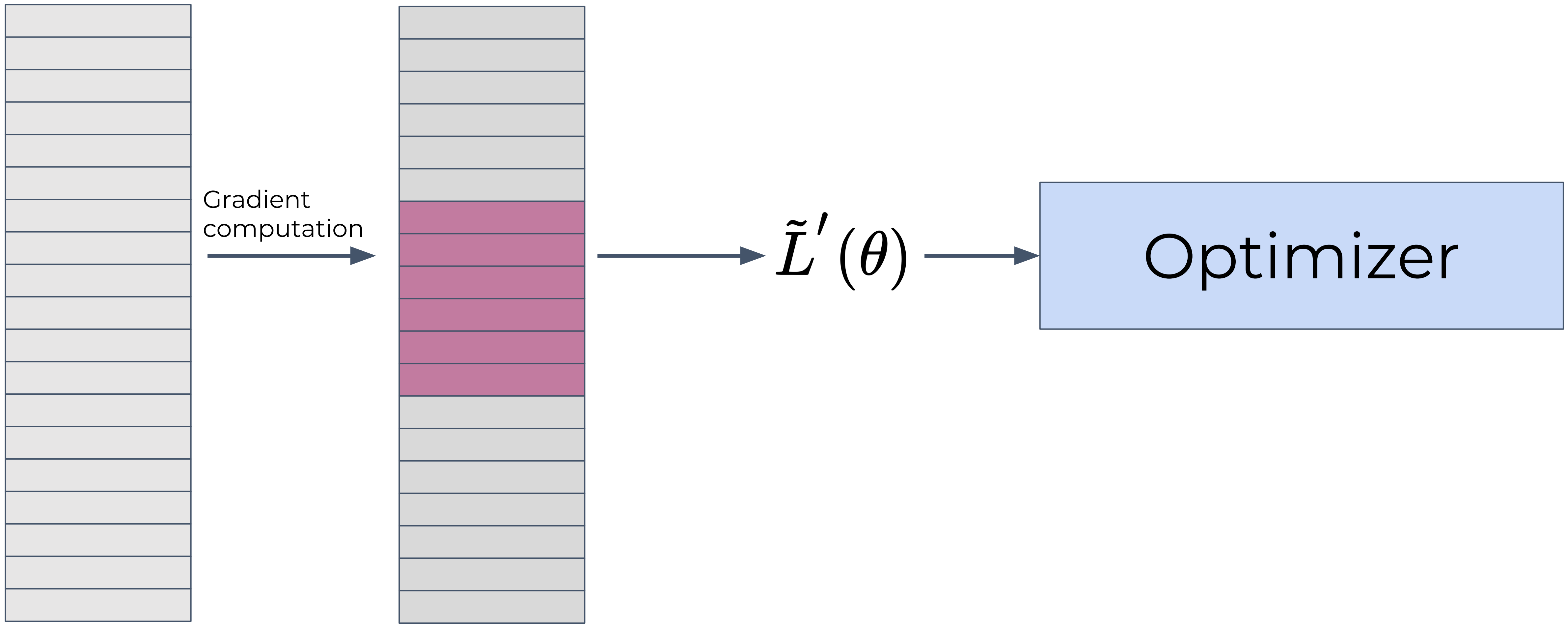
Gradient descent



Stochastic gradient descent



Stochastic gradient descent



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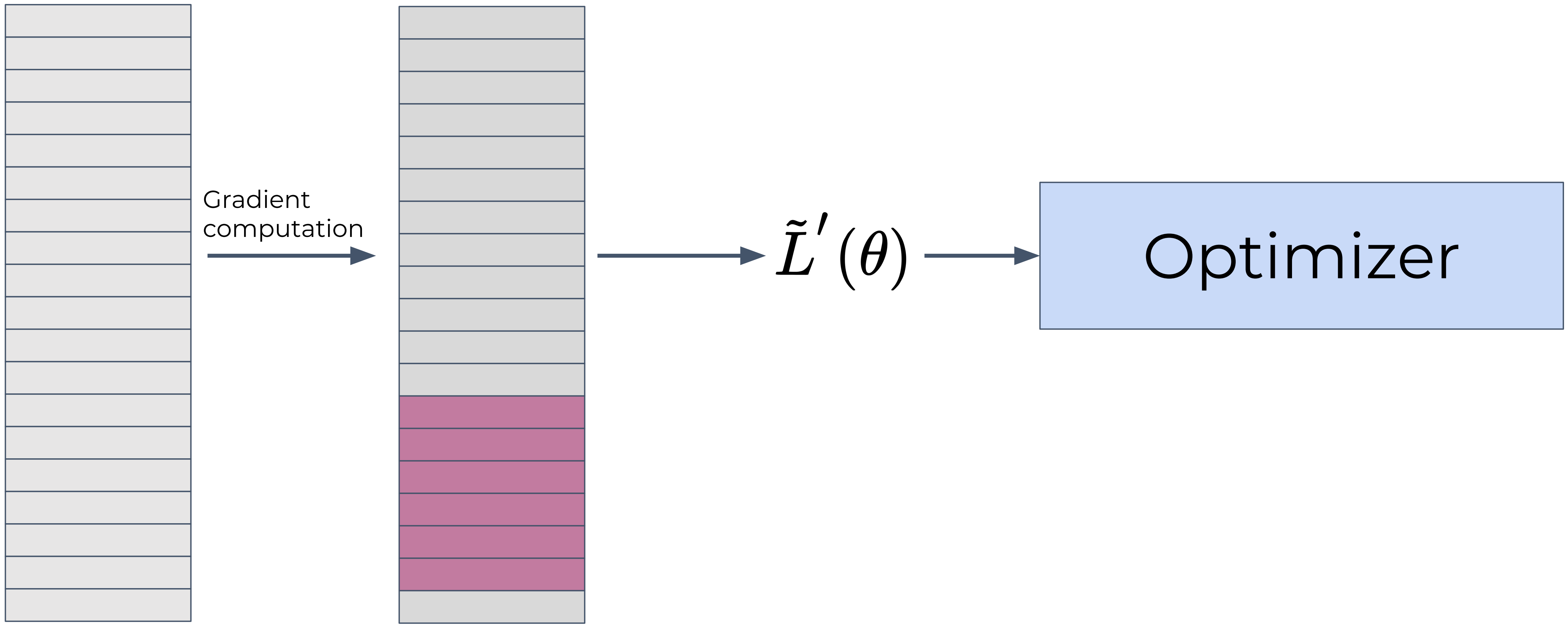

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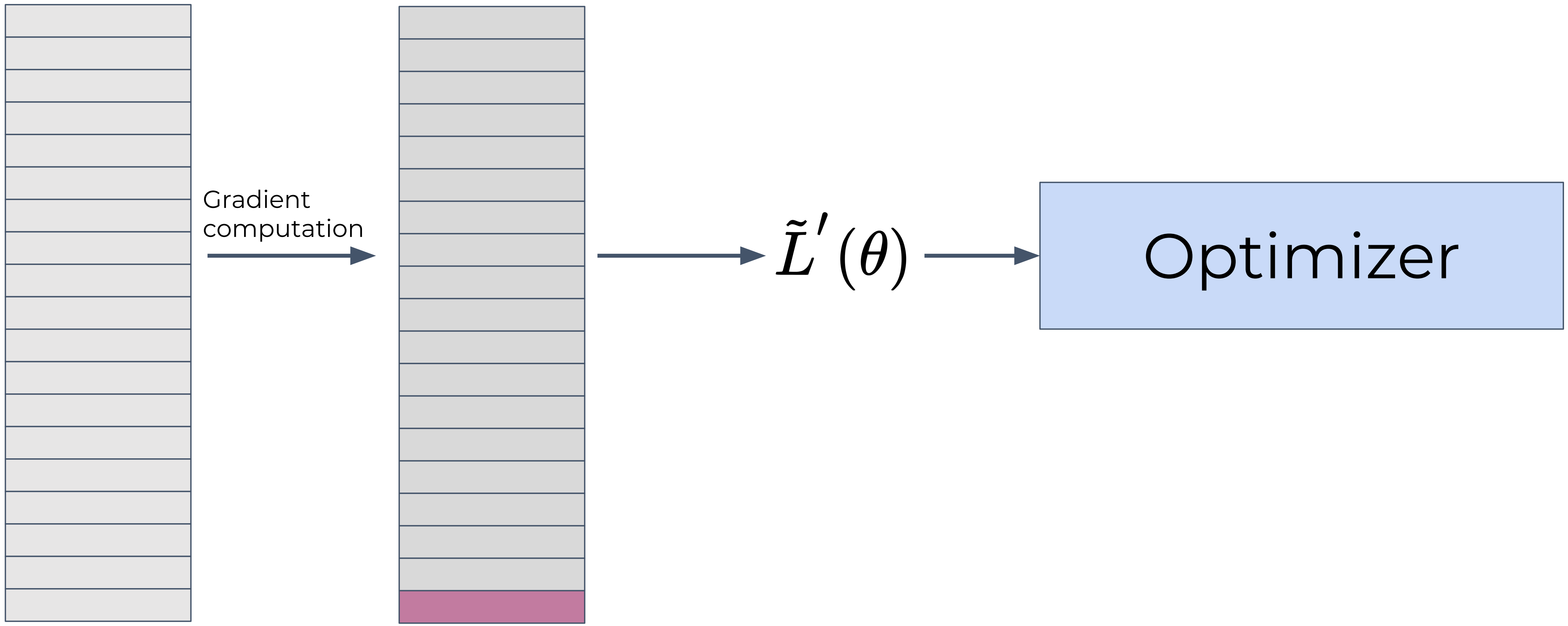

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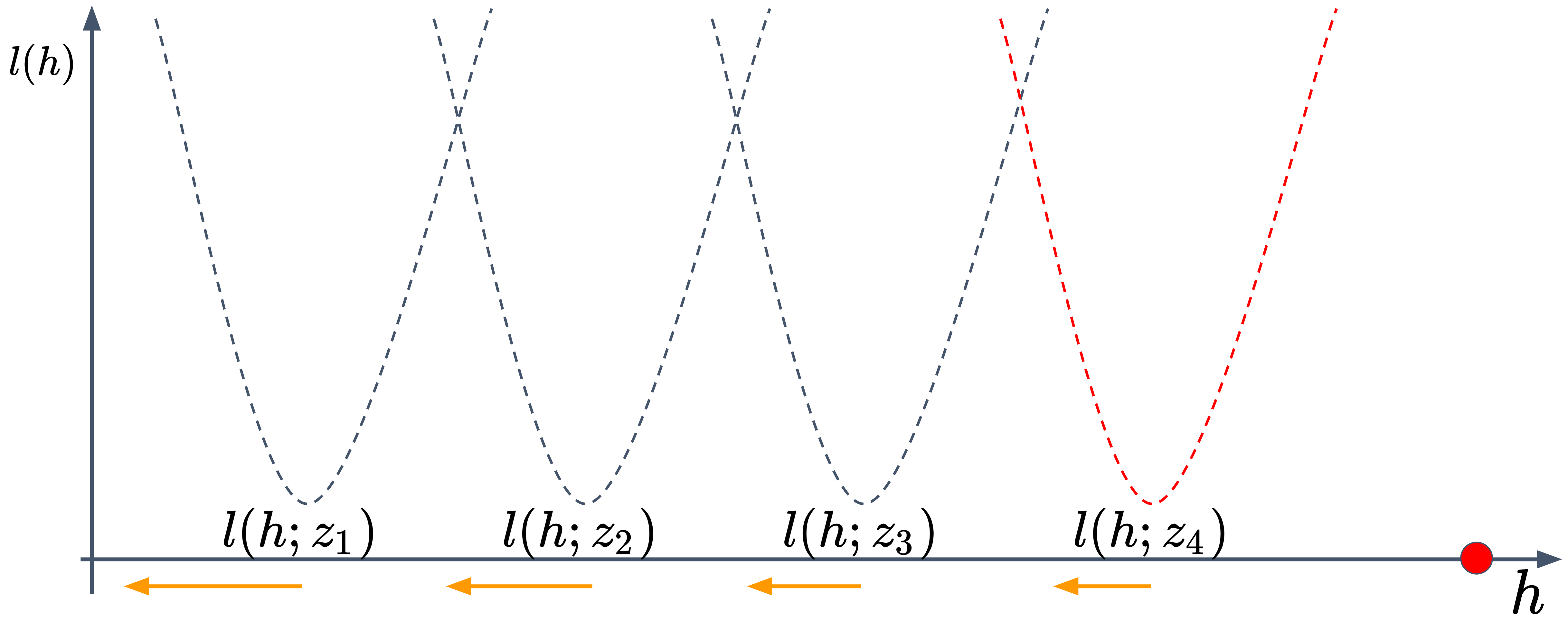
Convergence problem



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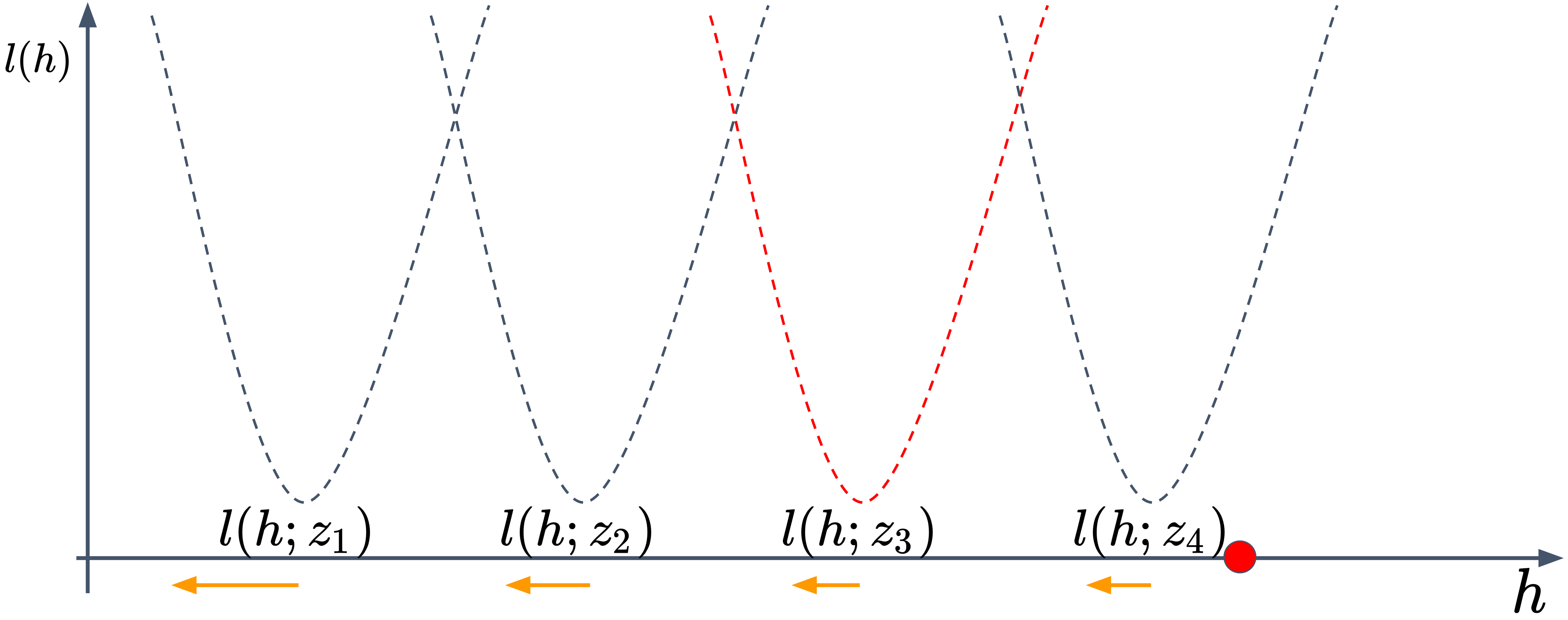

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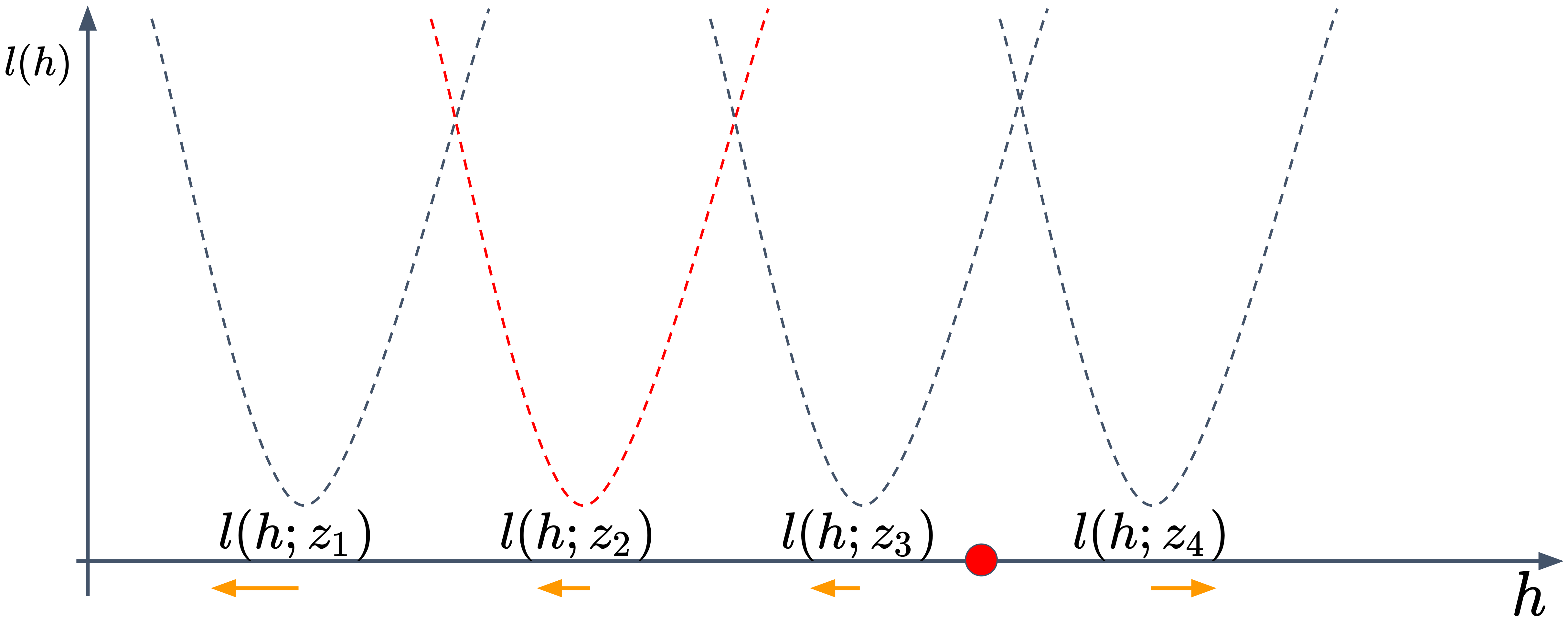

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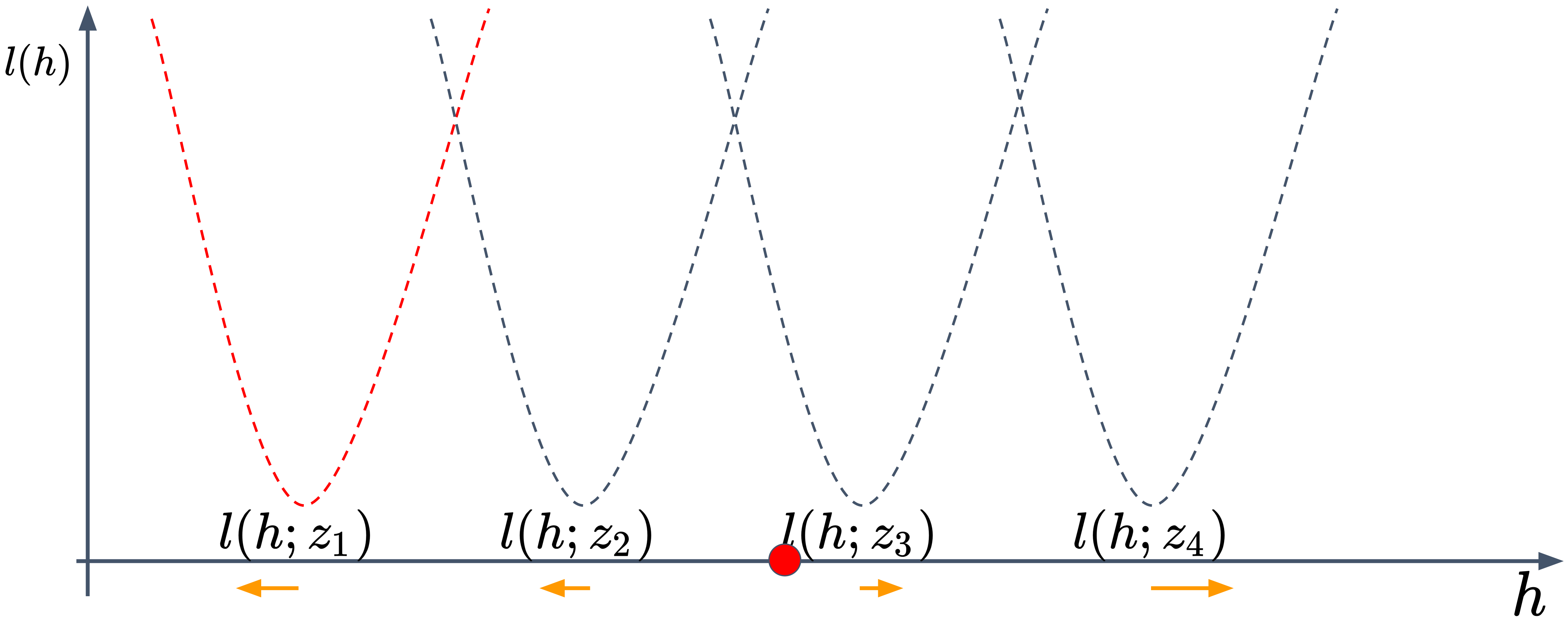

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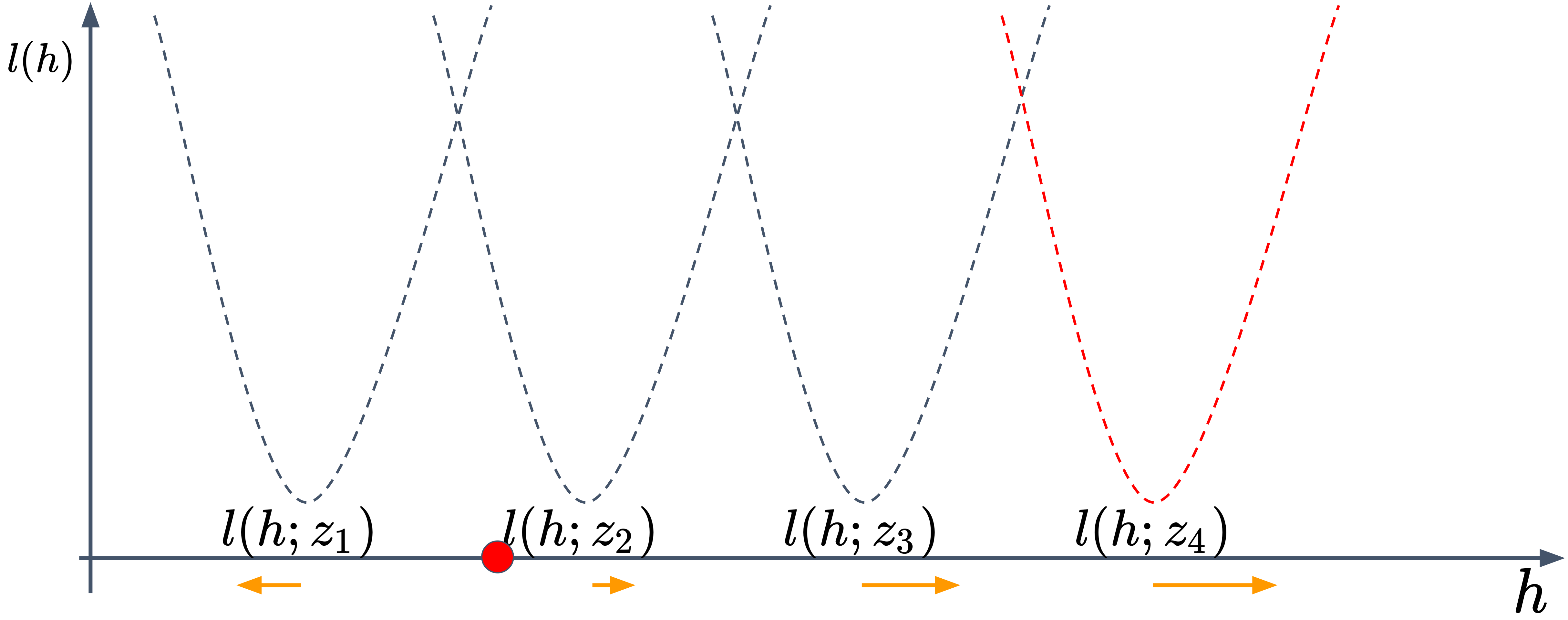

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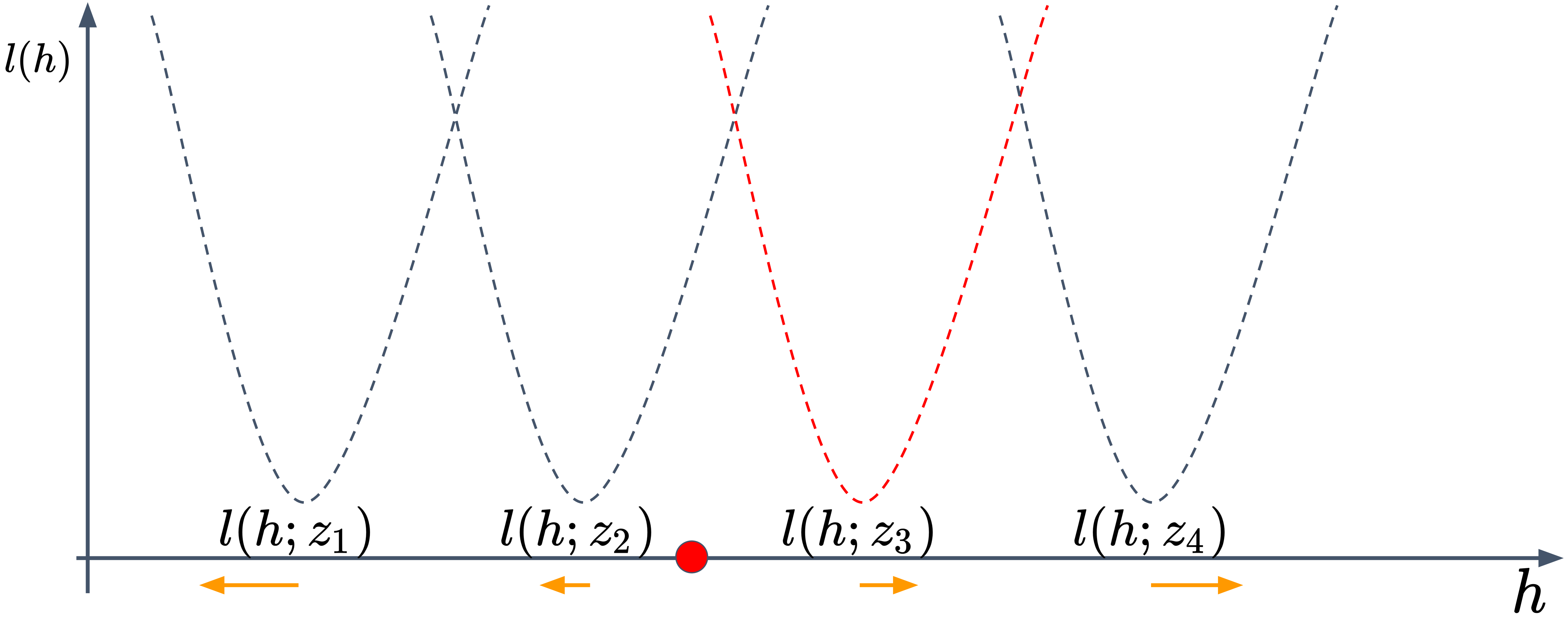

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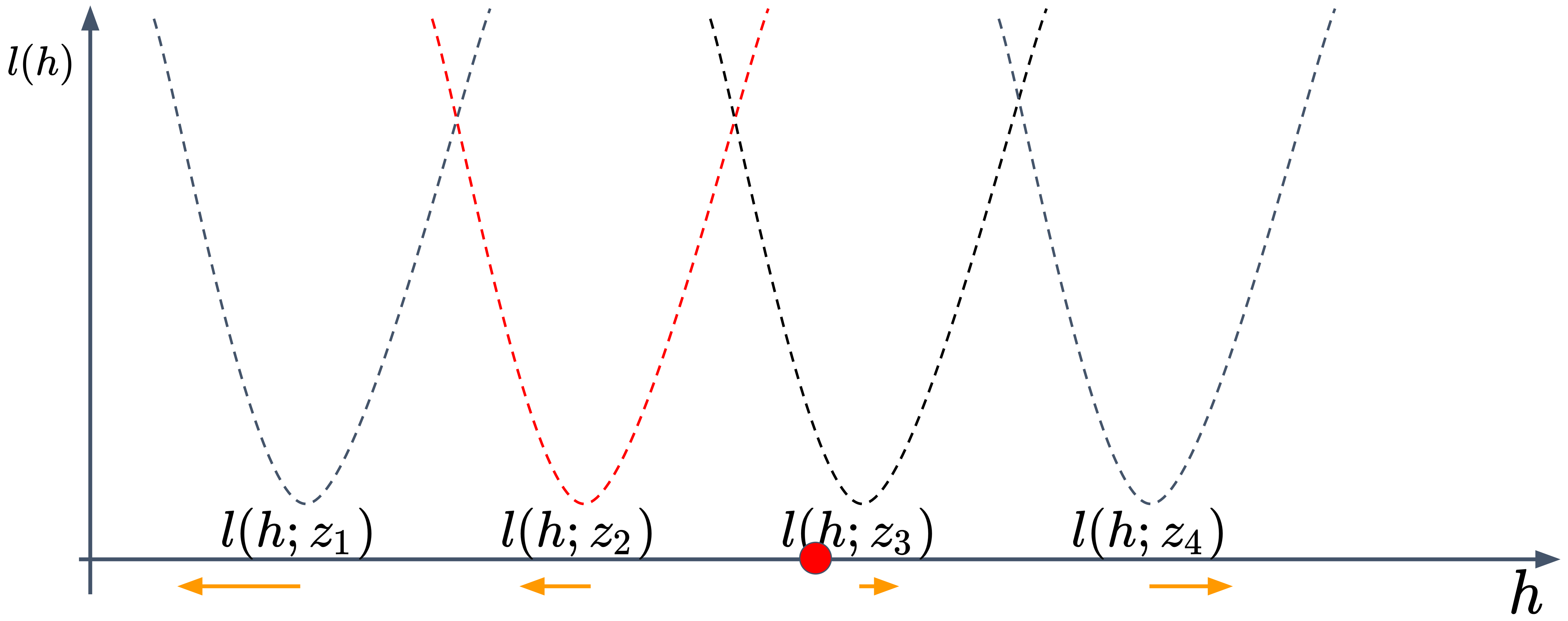
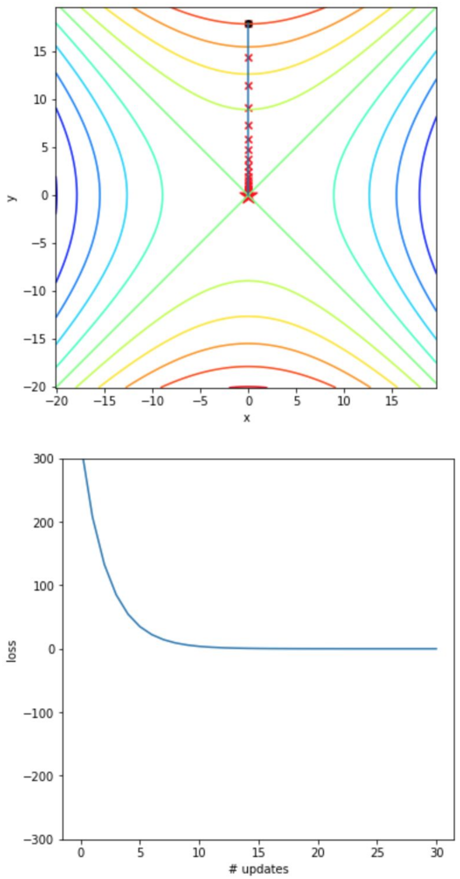
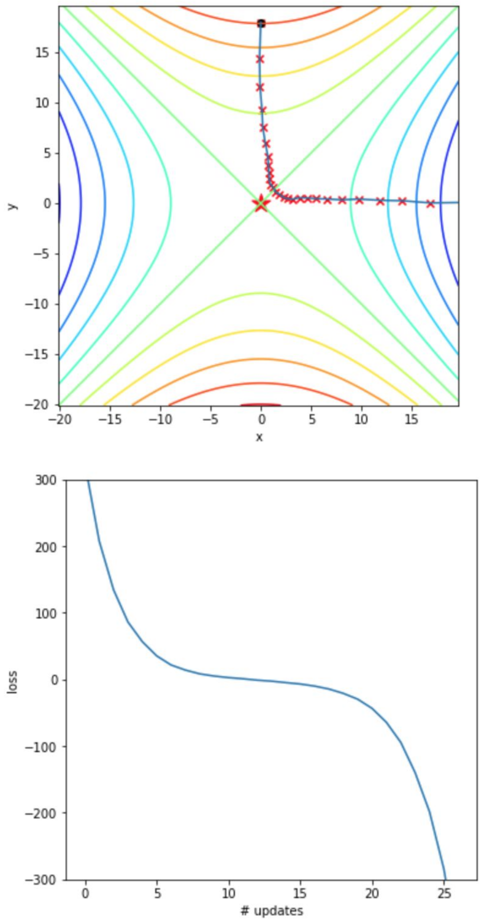
Convergence problem



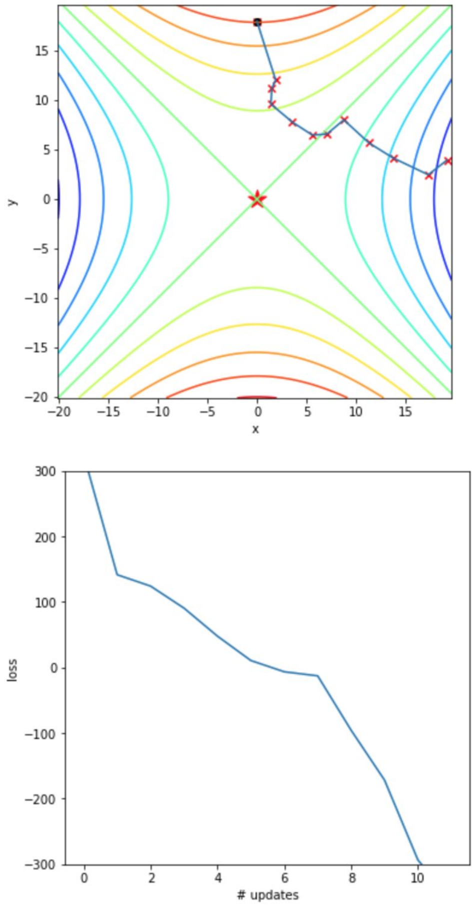
Escape the saddle points



$$\sigma^2 = 0$$



$$\sigma^2 = 0.1$$



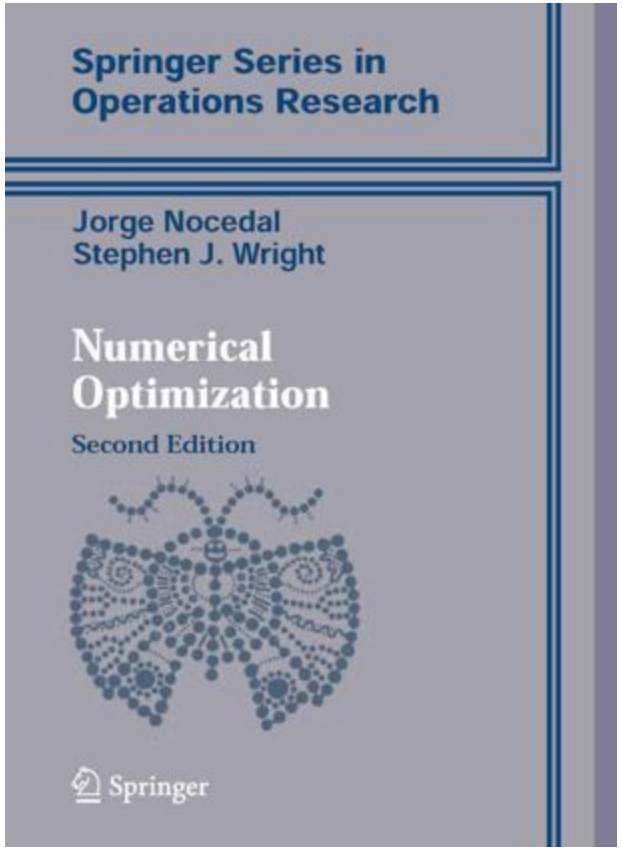
$$\sigma^2 = 1$$

Take-home message

- Machine learning is not only about optimization.
- Preconditioning facilitates optimization.
- Momentum leads to better results.
- Noise can have a beneficial effect for escaping saddle points.

References

- Explanation of the effect of noise on saddle points
- Explanation of the effect of momentum
- The chapter on numerical calculations in the book
  Deep Learning by Goodfellow, Bengio and Courville
- Explanation of Adam by Andrew Ng
- How to reduce learning rate by Andrew Ng
- Description of the different optimizers in DL



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