CM20315 - Machine Learning

Prof. Simon Prince

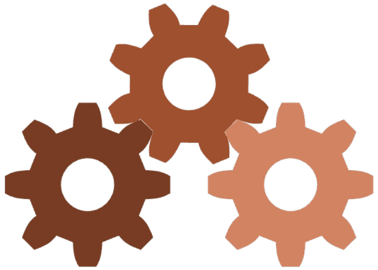
6. Fitting models

Regression

Real world input | Model input | Model | Model output | Real world output

6000 square feet,
4 bedrooms,
previously sold for
$235K in 2005,
1 parking spot.

→ $\begin{bmatrix}6000\\4\\235\\2005\\1\end{bmatrix}$ →



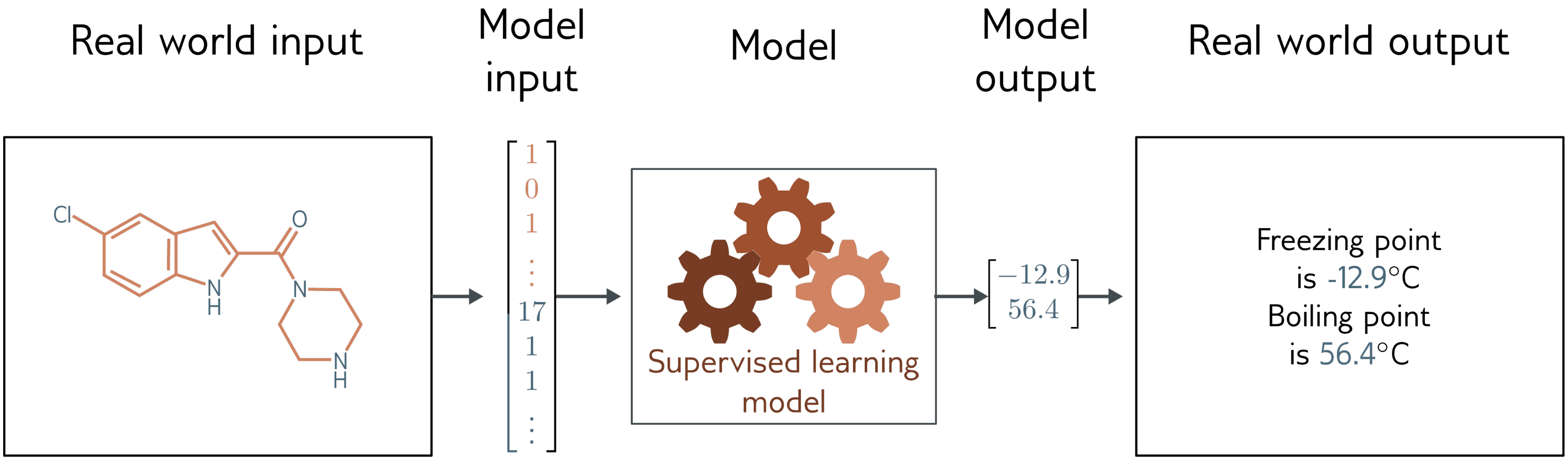
Supervised learning model

→ $[340]$ →

Predicted price
is $340k

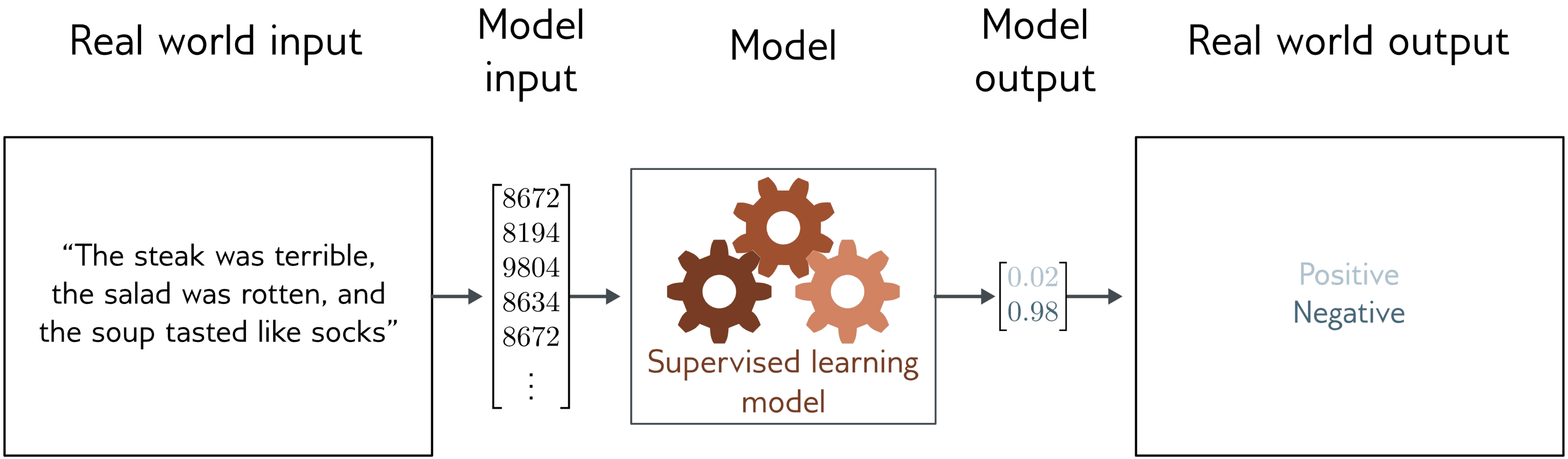
- Univariate regression problem (one output, real value

Graph regression



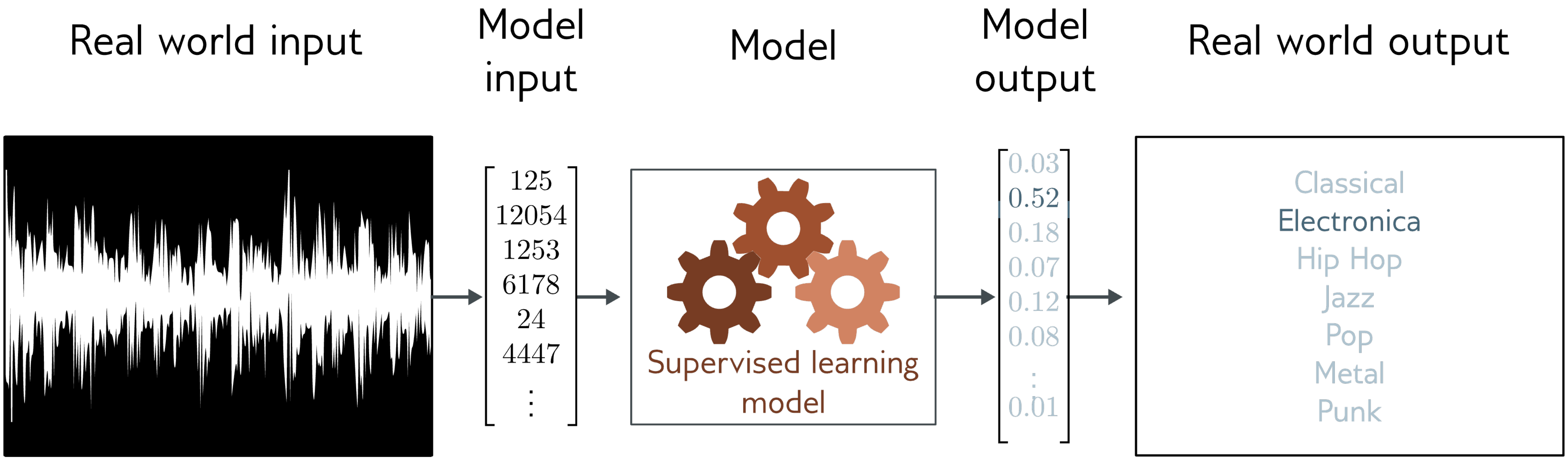
- Multivariate regression problem (>1 output, real value)

Text classification



- Binary classification problem (two discrete classes)

Music genre classification



- Multiclass classification problem (discrete classes, >2 possible values)

Loss function

- Training dataset of I pairs of input/output examples:

$$\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{I}$$

- Loss function or cost function measures how bad model is:

$$L[\phi, \mathrm{f}[\mathbf{x}_i, \phi], \{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{I}]$$

or for short:

$$L[\phi]$$

Returns a scalar that is smaller when model maps inputs to outputs better

Training

- Loss function:

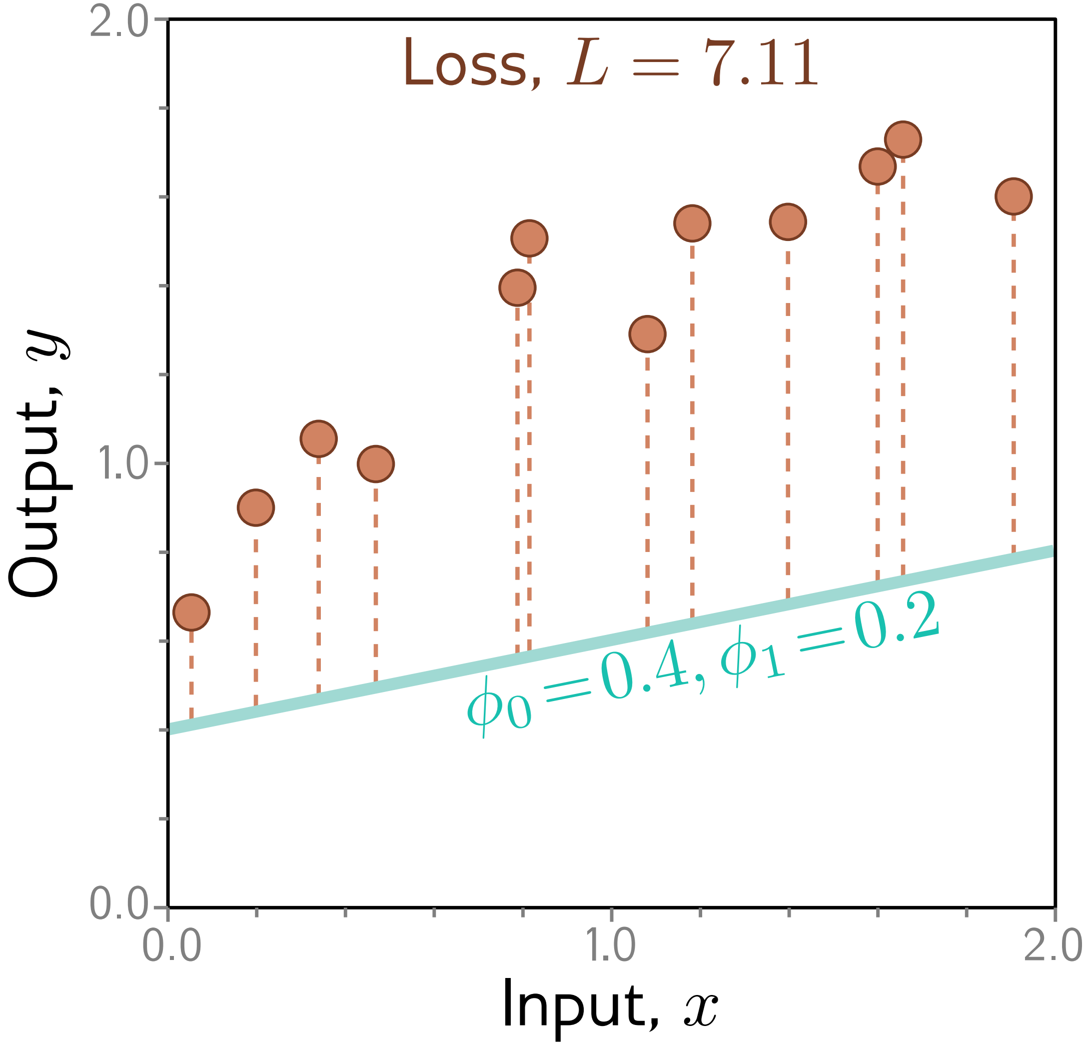
$$L[\phi]$$

Returns a scalar that is smaller when model maps inputs to outputs better

- Find the parameters that minimize the loss:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}}\left[L[\phi]\right]$$

Example: 1D Linear regression loss function



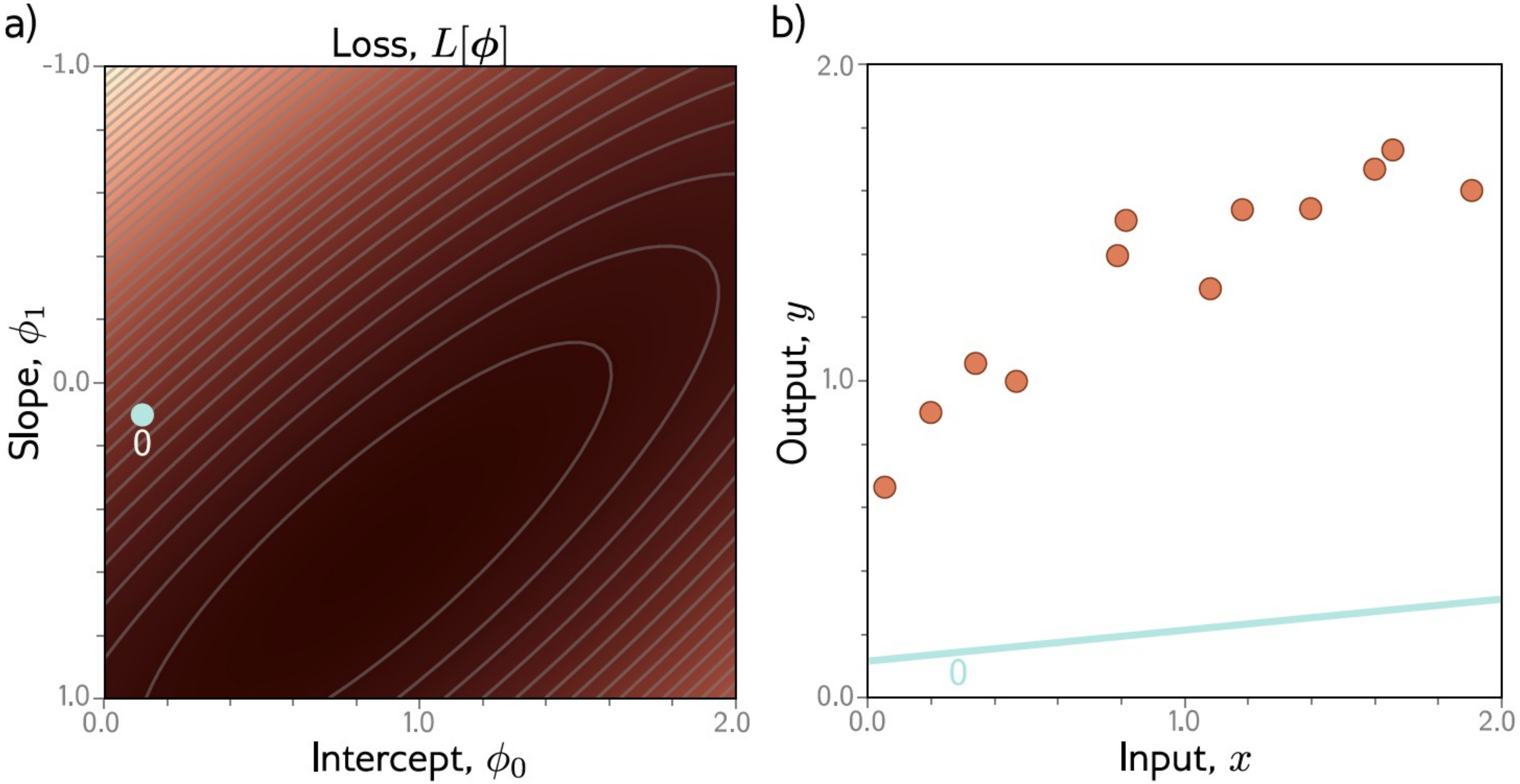
Loss function:

$$L[\boldsymbol{\phi}] = \sum_{i=1}^{I} (\text{f}[x_i, \boldsymbol{\phi}] - y_i)^2$$

$$= \sum_{i=1}^{I} (\phi_0 + \phi_1 x_i - y_i)^2$$

"Least squares loss function"

Example: 1D Linear regression training



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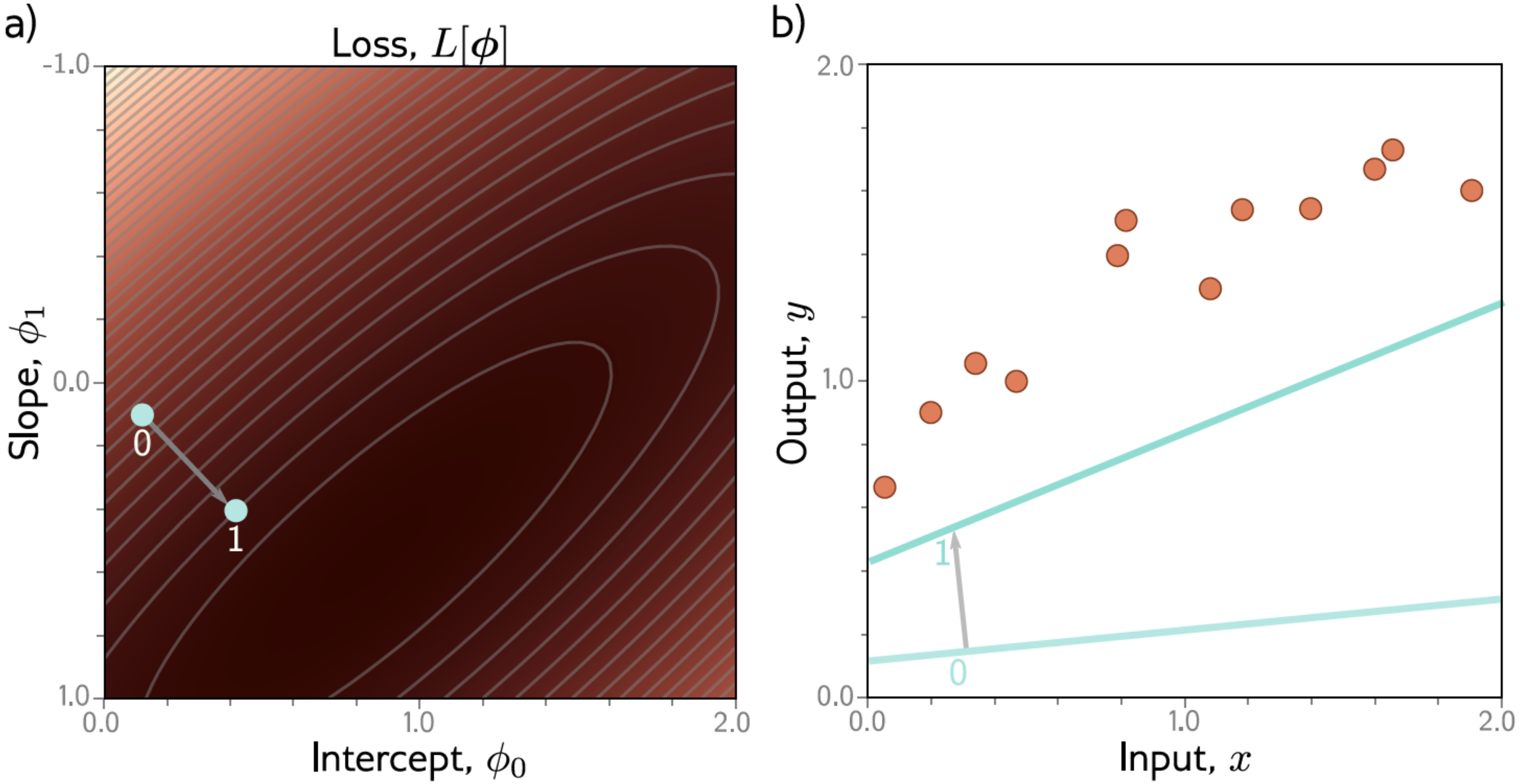

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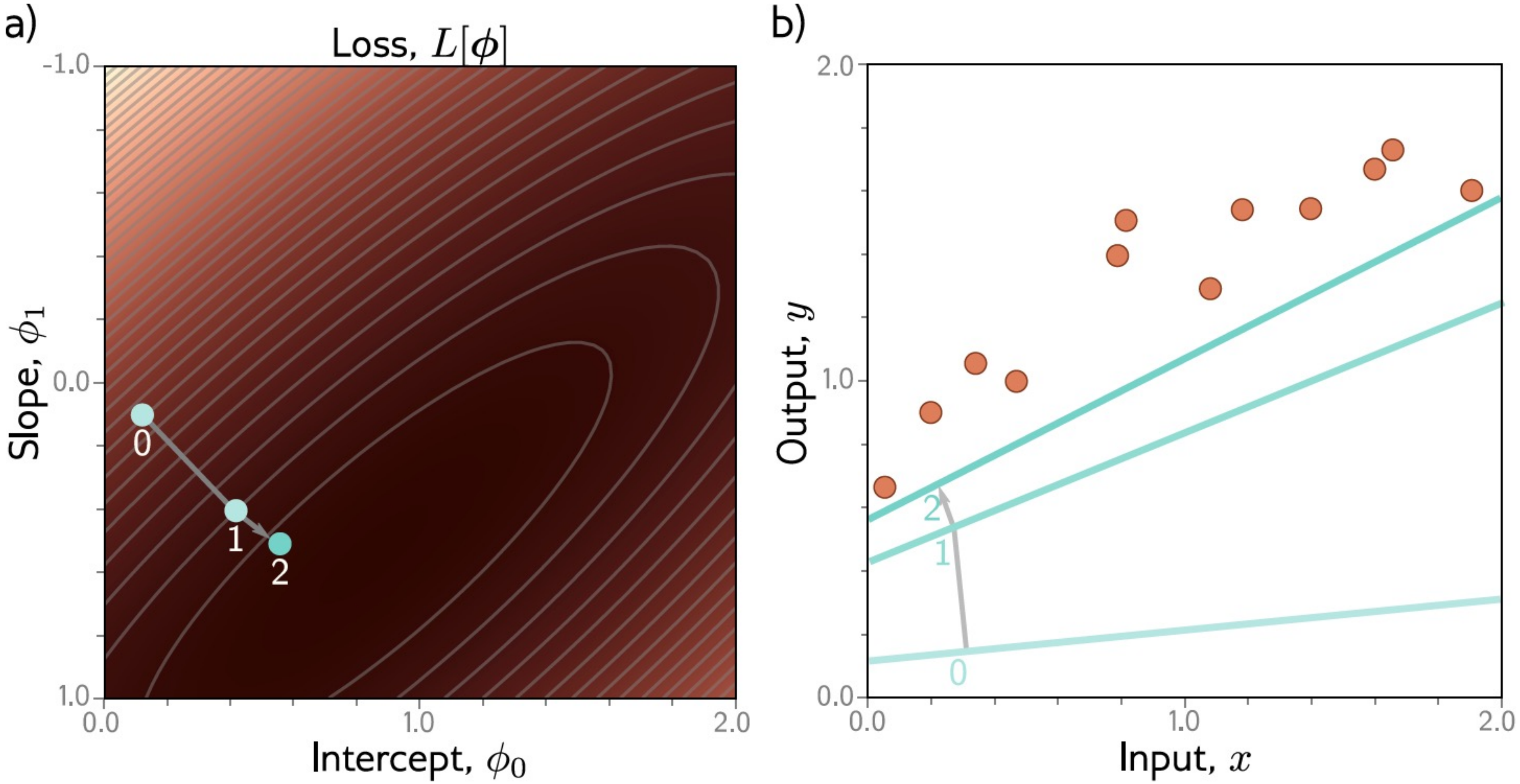

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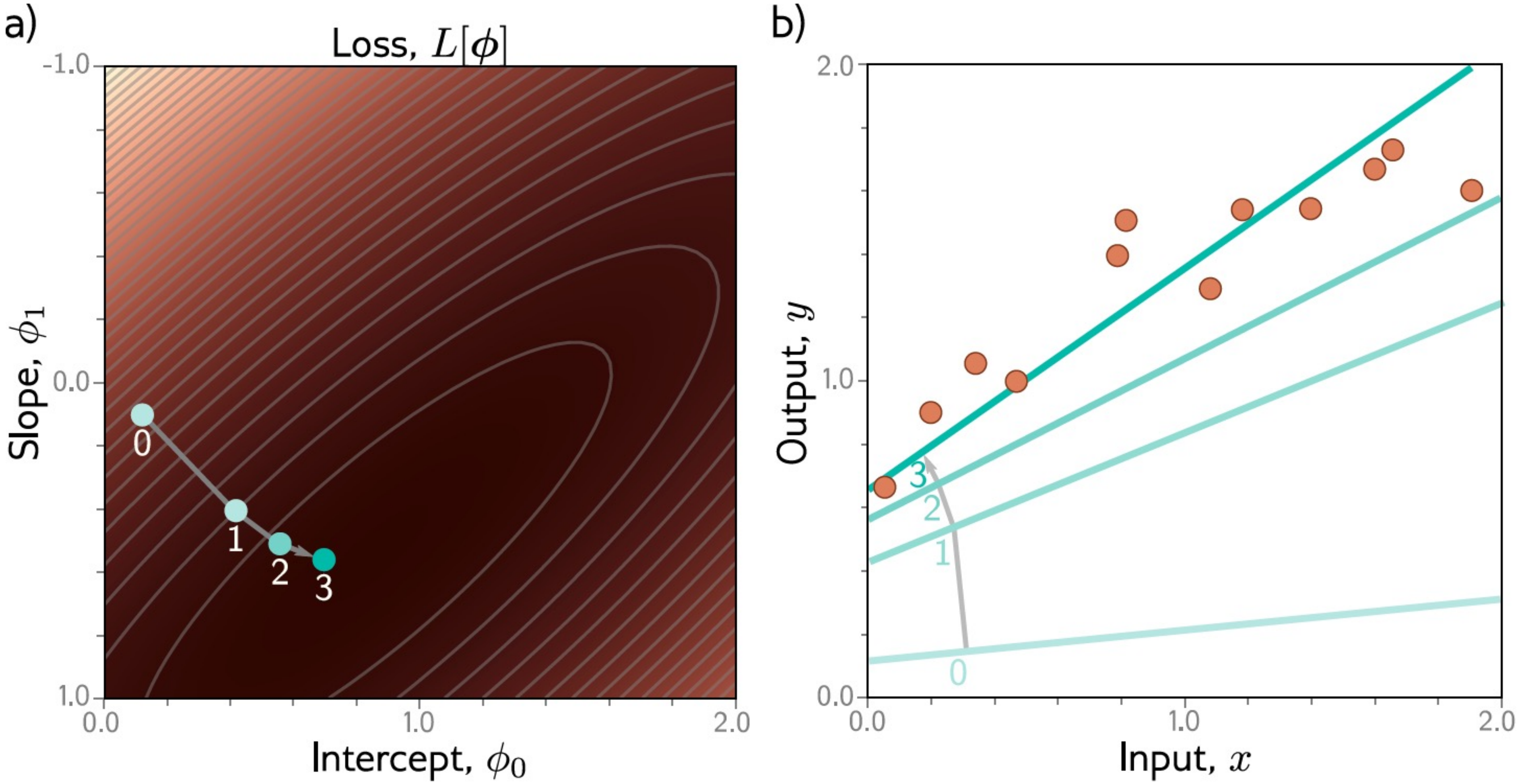

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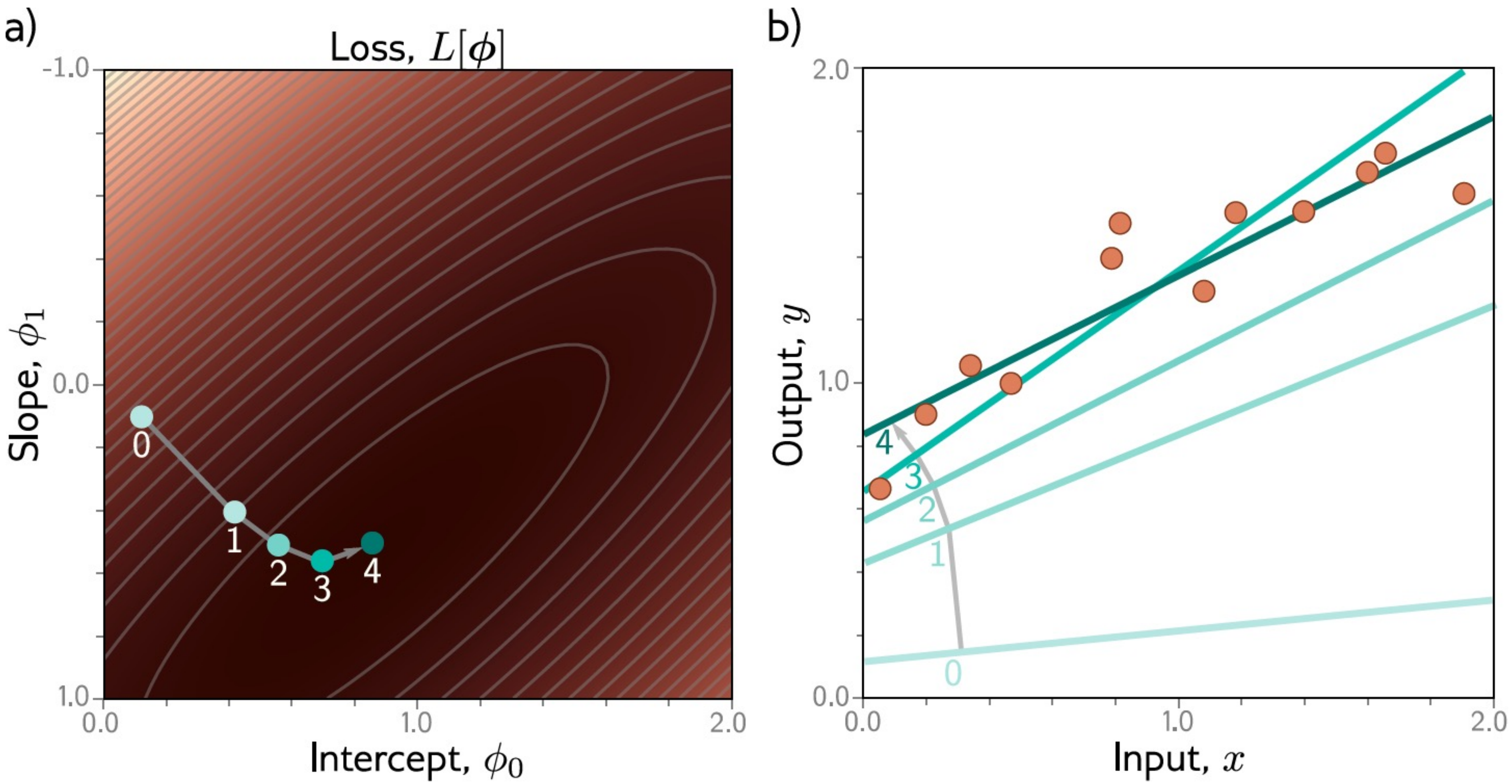
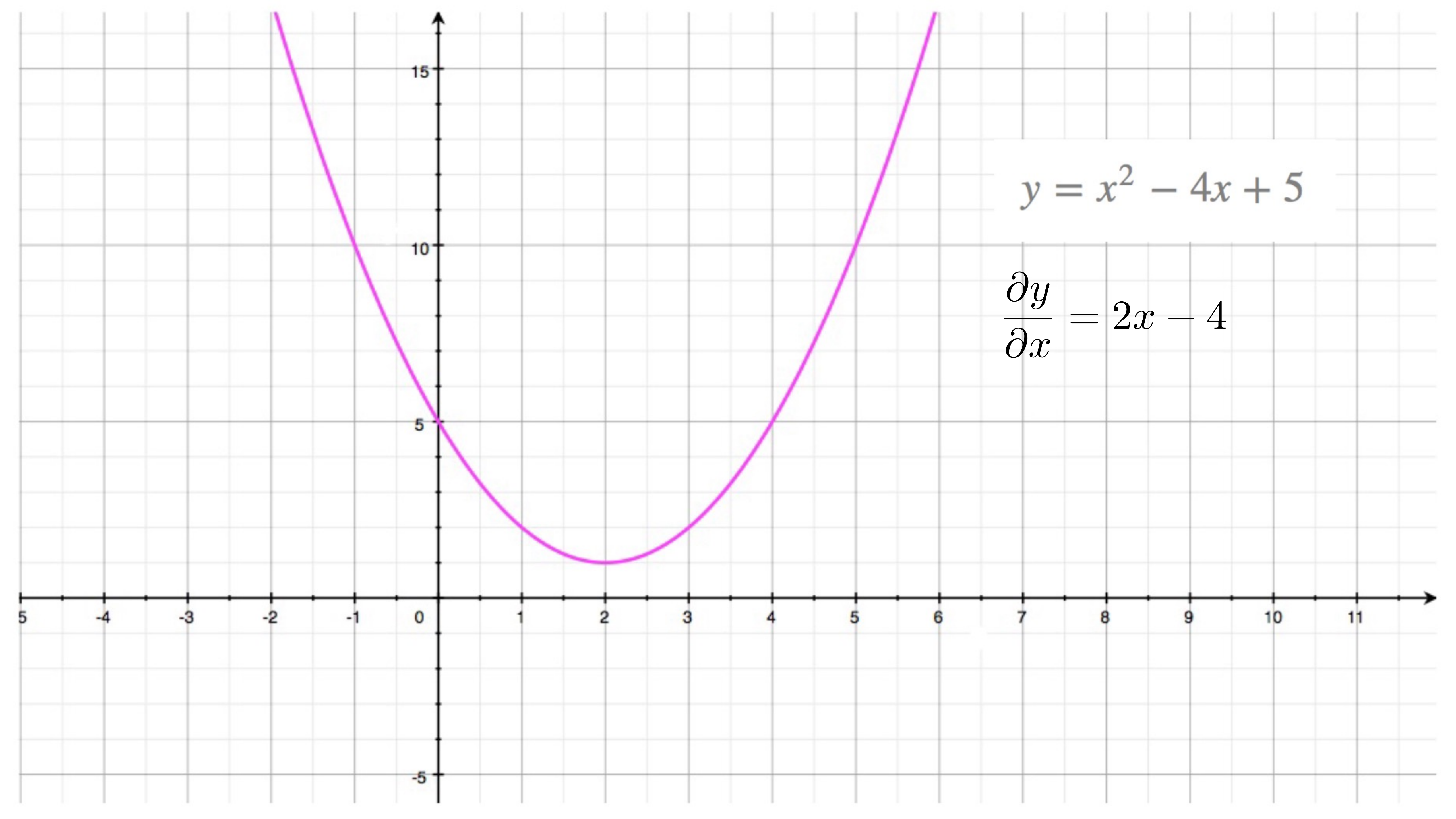


This technique is known as gradient descent

Fitting models

- Maths overview
- Gradient descent algorithm
- Linear regression example
- Gabor model example
- Stochastic gradient descent
- Momentum
- Adam



y = x^2 - 4x + 5
∂y/∂x = 2x - 4
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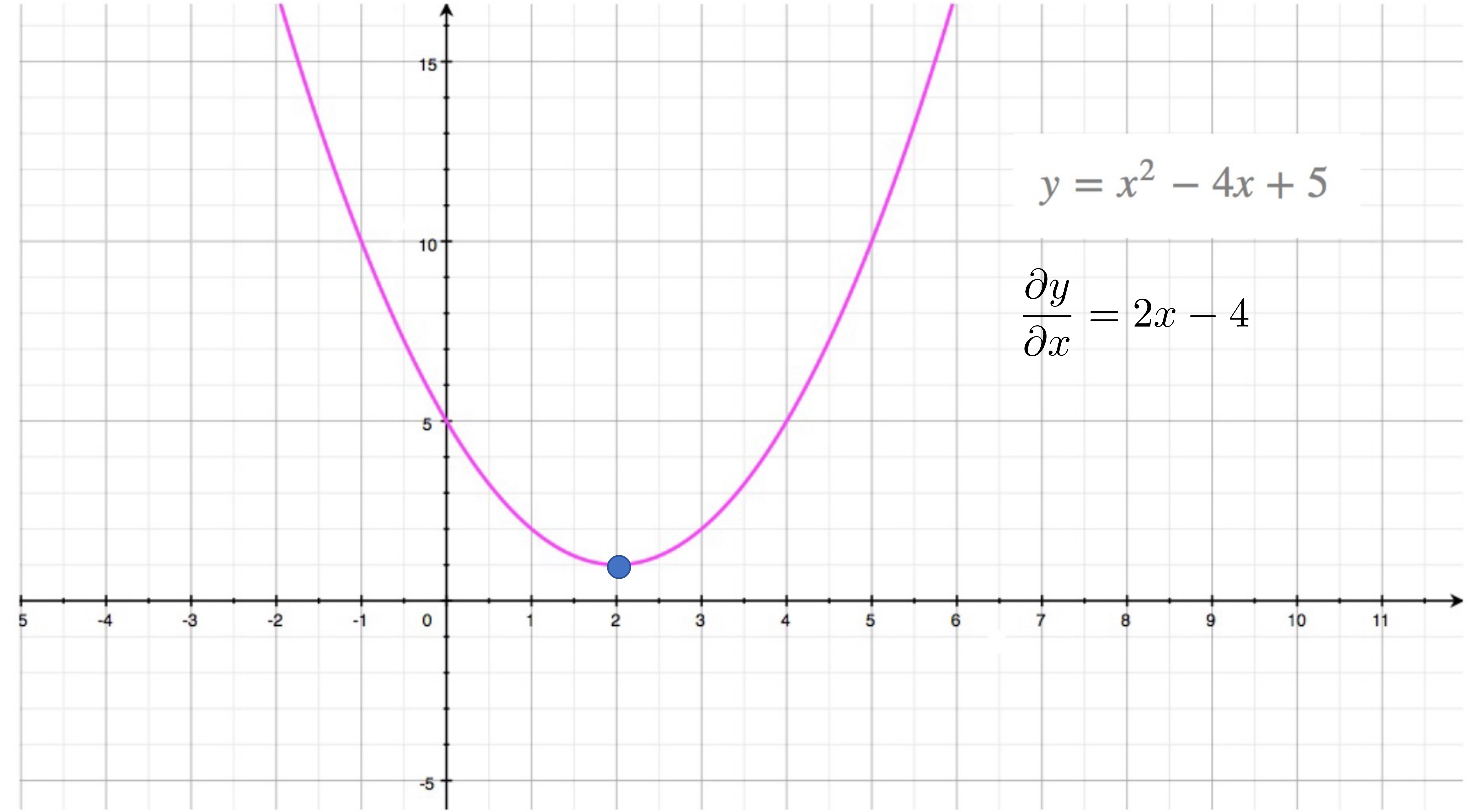

$y = x^2 - 4x + 5$
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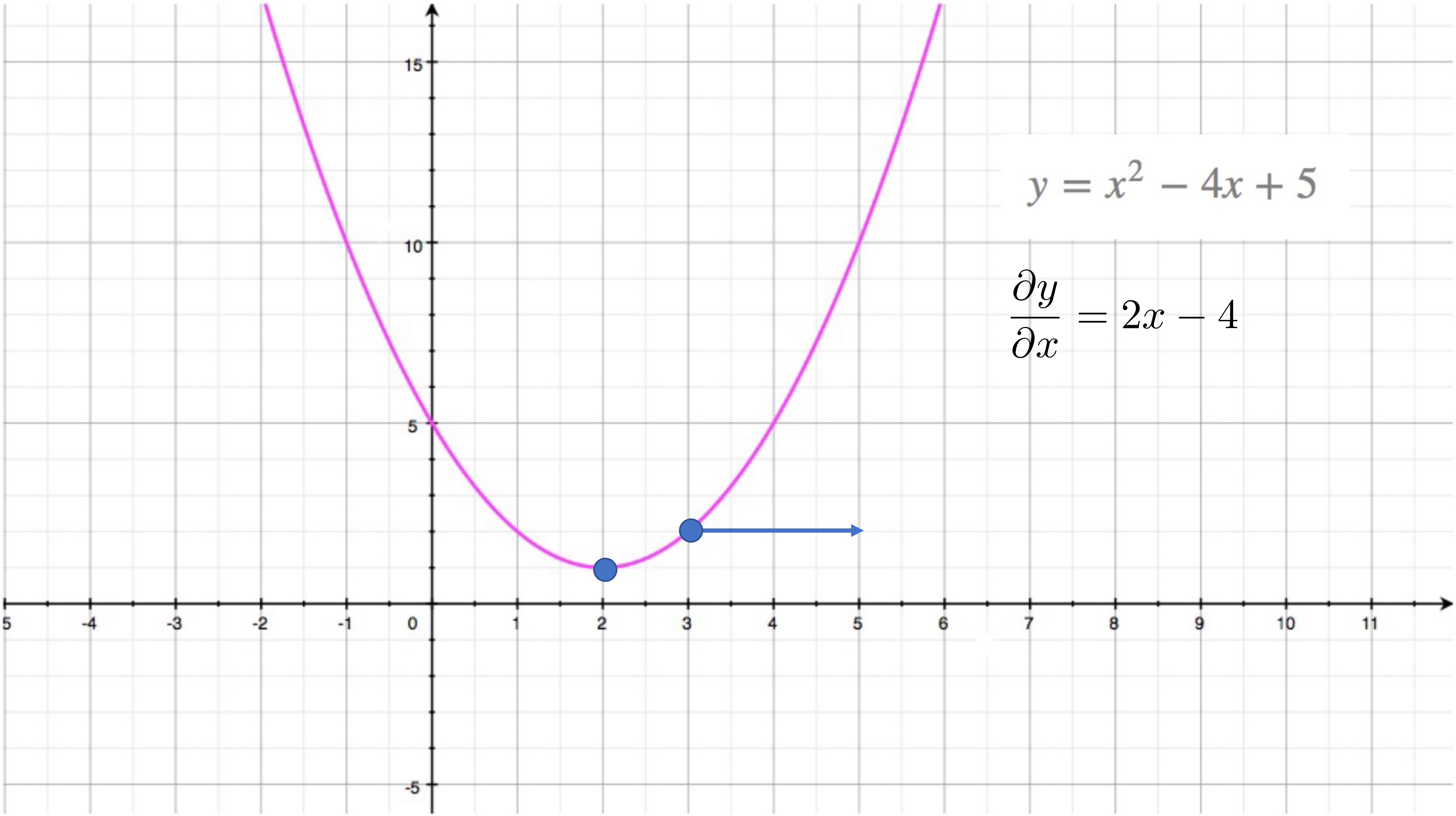

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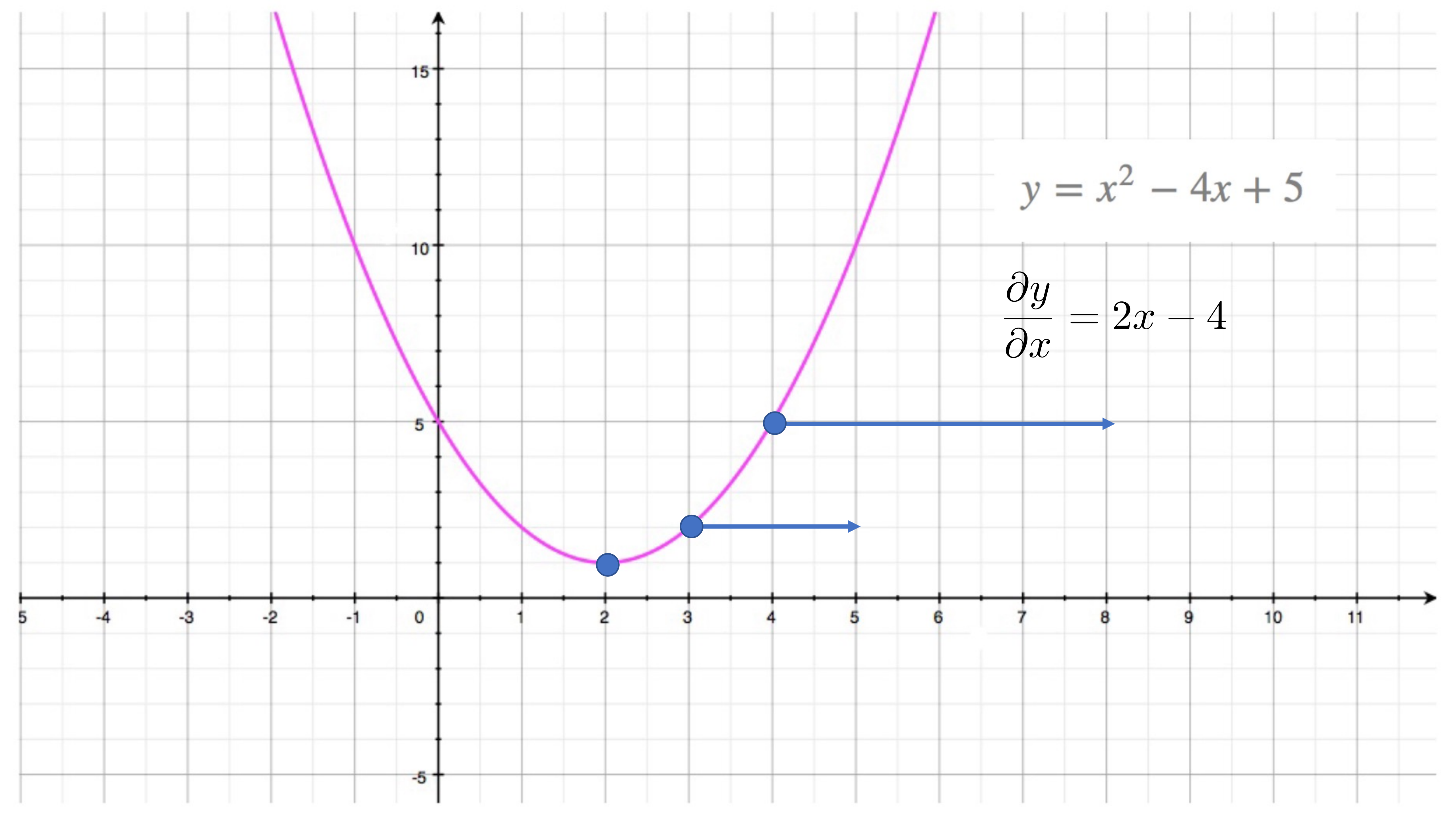

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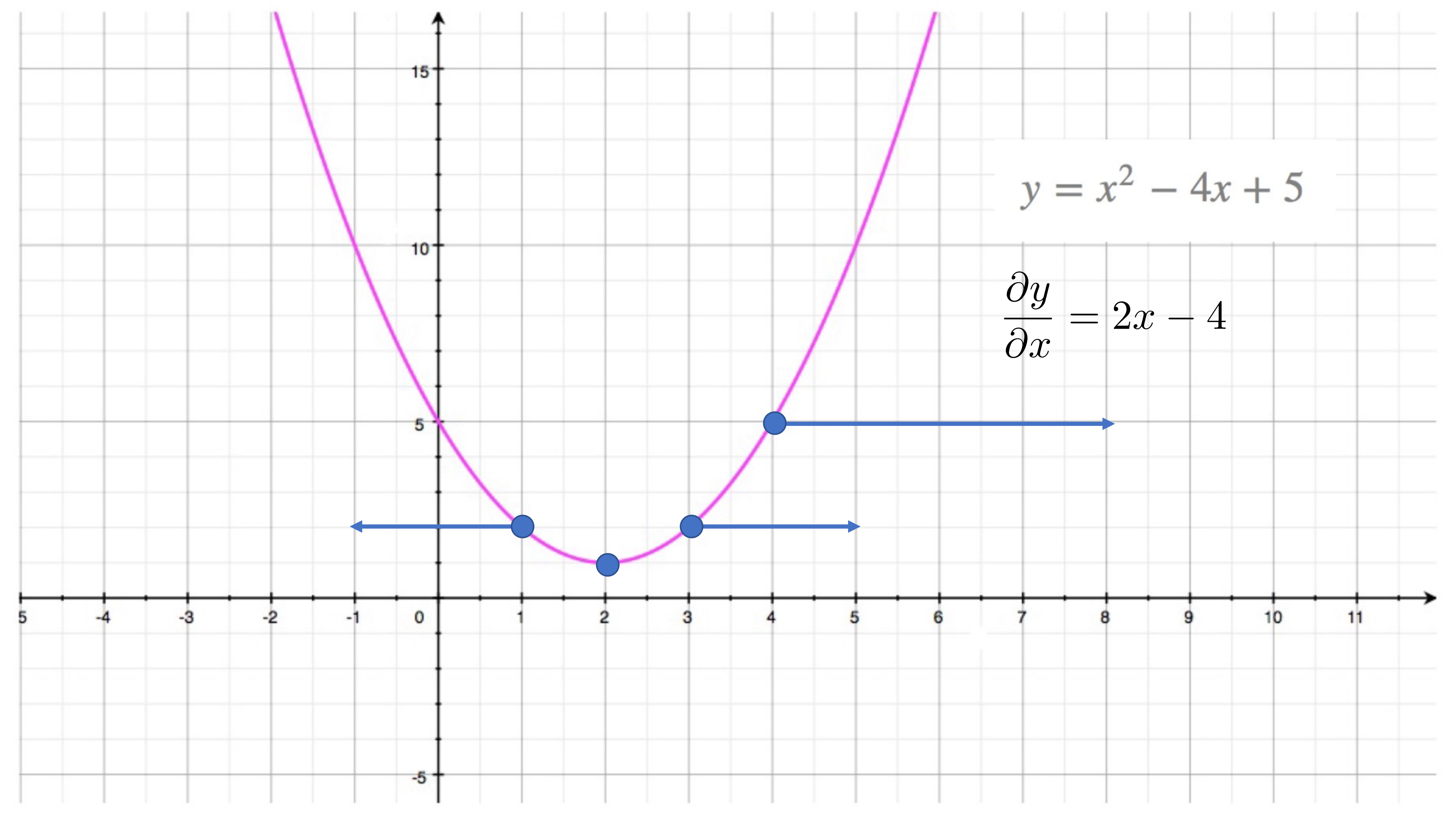

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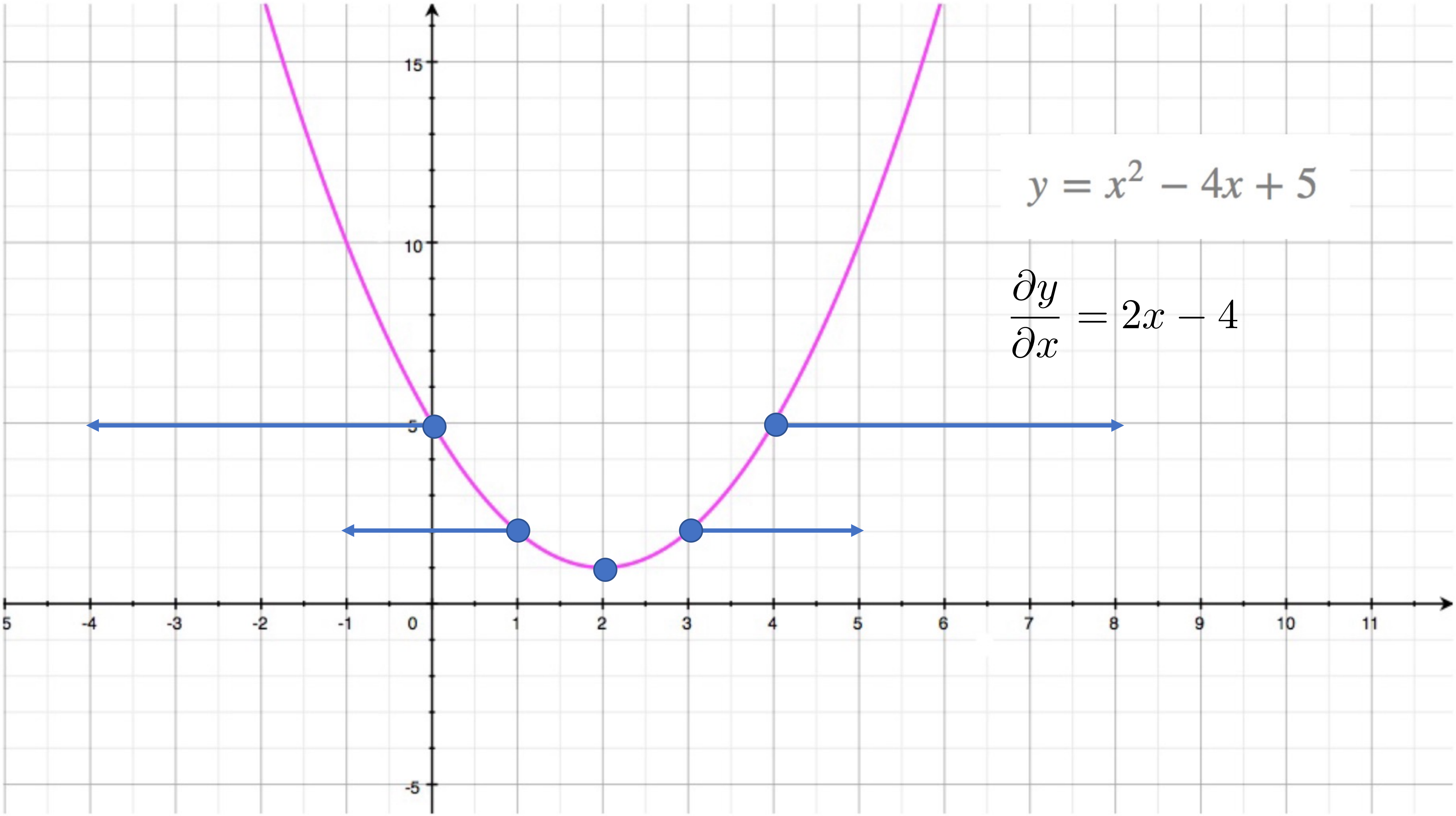
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Gradient descent algorithm

Step 1. Compute the derivatives of the loss with respect to the parameters:

$$\frac{\partial L}{\partial \phi} = \begin{bmatrix} \frac{\partial L}{\partial \phi_0} \\ \frac{\partial L}{\partial \phi_1} \\ \vdots \\ \frac{\partial L}{\partial \phi_N} \end{bmatrix}.$$

Step 2. Update the parameters according to the rule:

$$\phi \longleftarrow \phi - \alpha \frac{\partial L}{\partial \phi},$$

where the positive scalar α determines the magnitude of the change.

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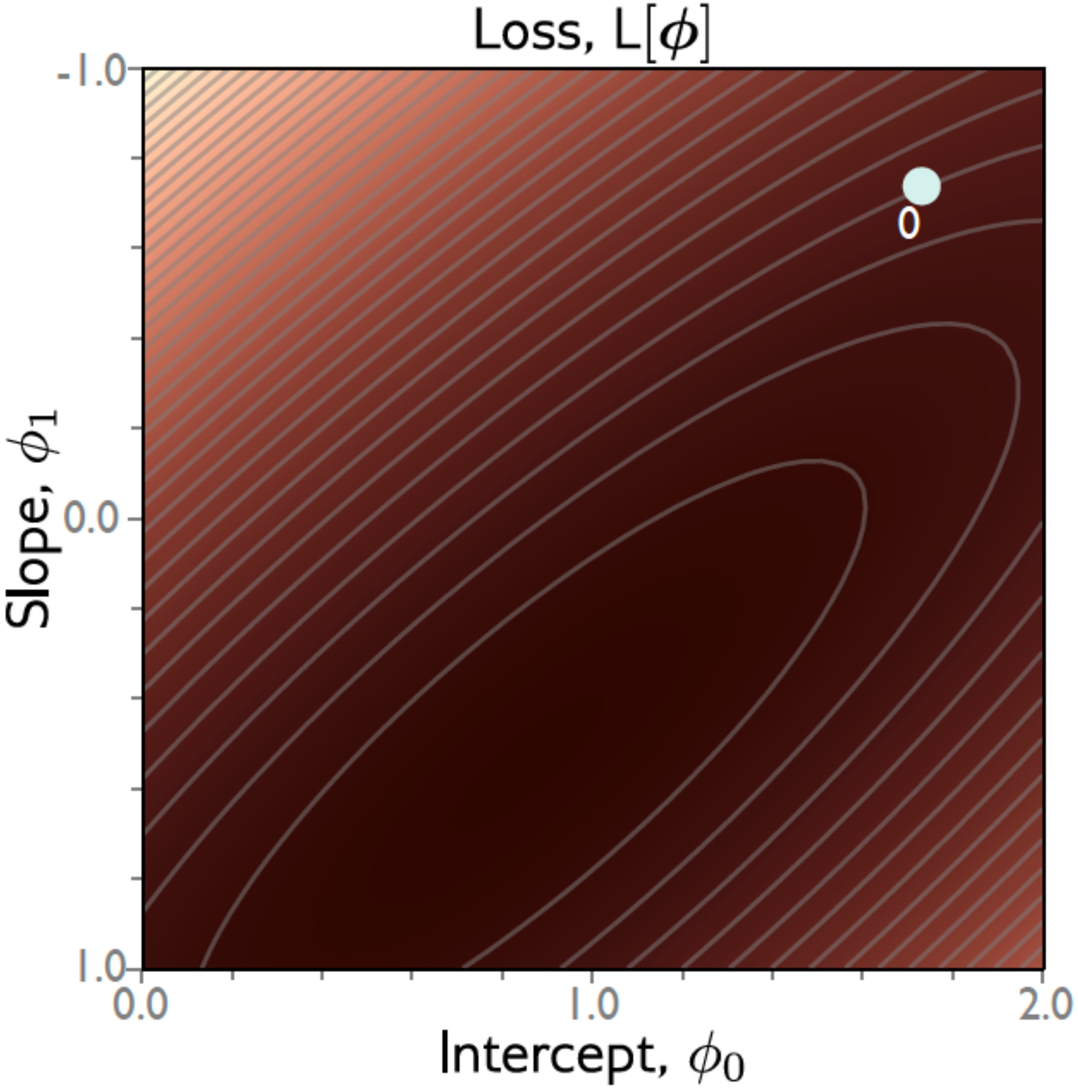
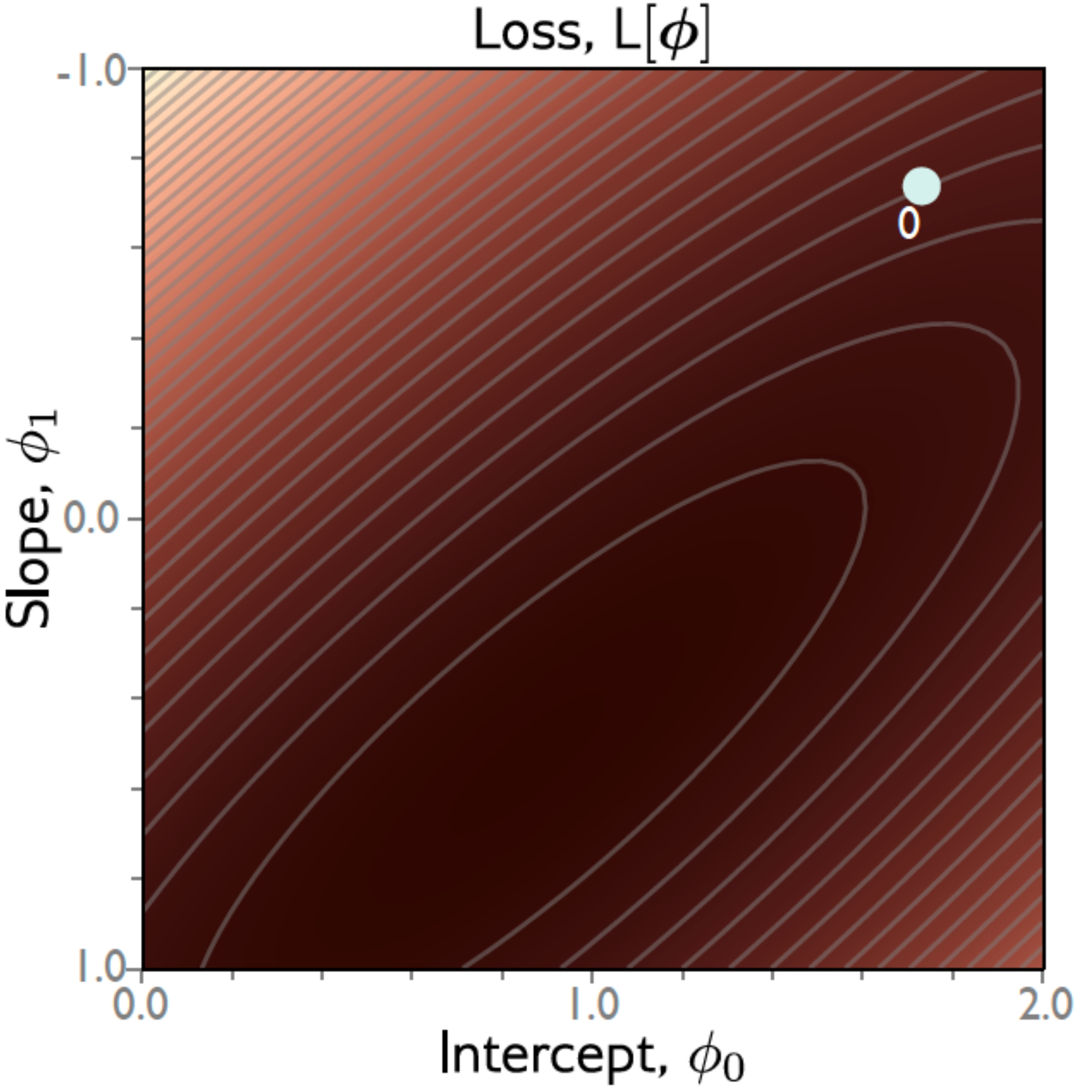
Gradient descent



Step 1: Compute derivatives (slopes of function) with Respect to the parameters

$$
\begin{aligned}
L[\phi] &= \sum_{i=1}^{I} \ell_i = \sum_{i=1}^{I} \left(\mathrm{f}[x_i, \phi] - y_i\right)^2 \\
&= \sum_{i=1}^{I} \left(\phi_0 + \phi_1 x_i - y_i\right)^2
\end{aligned}
$$

Gradient descent



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\frac{\partial L}{\partial \phi} = \frac{\partial}{\partial \phi} \sum_{i=1}^{I} \ell_i = \sum_{i=1}^{I} \frac{\partial \ell_i}{\partial \phi}
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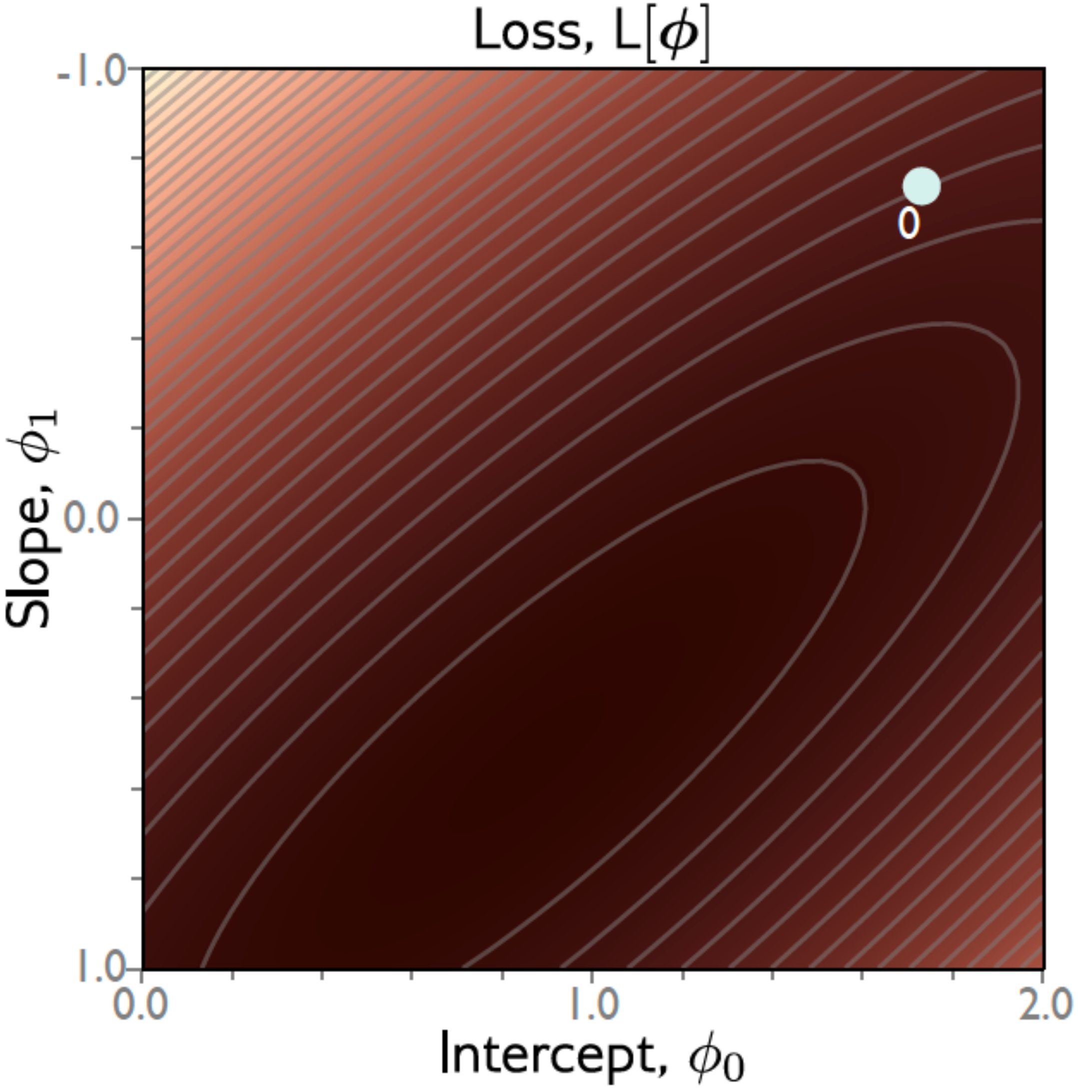
Gradient descent



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$$

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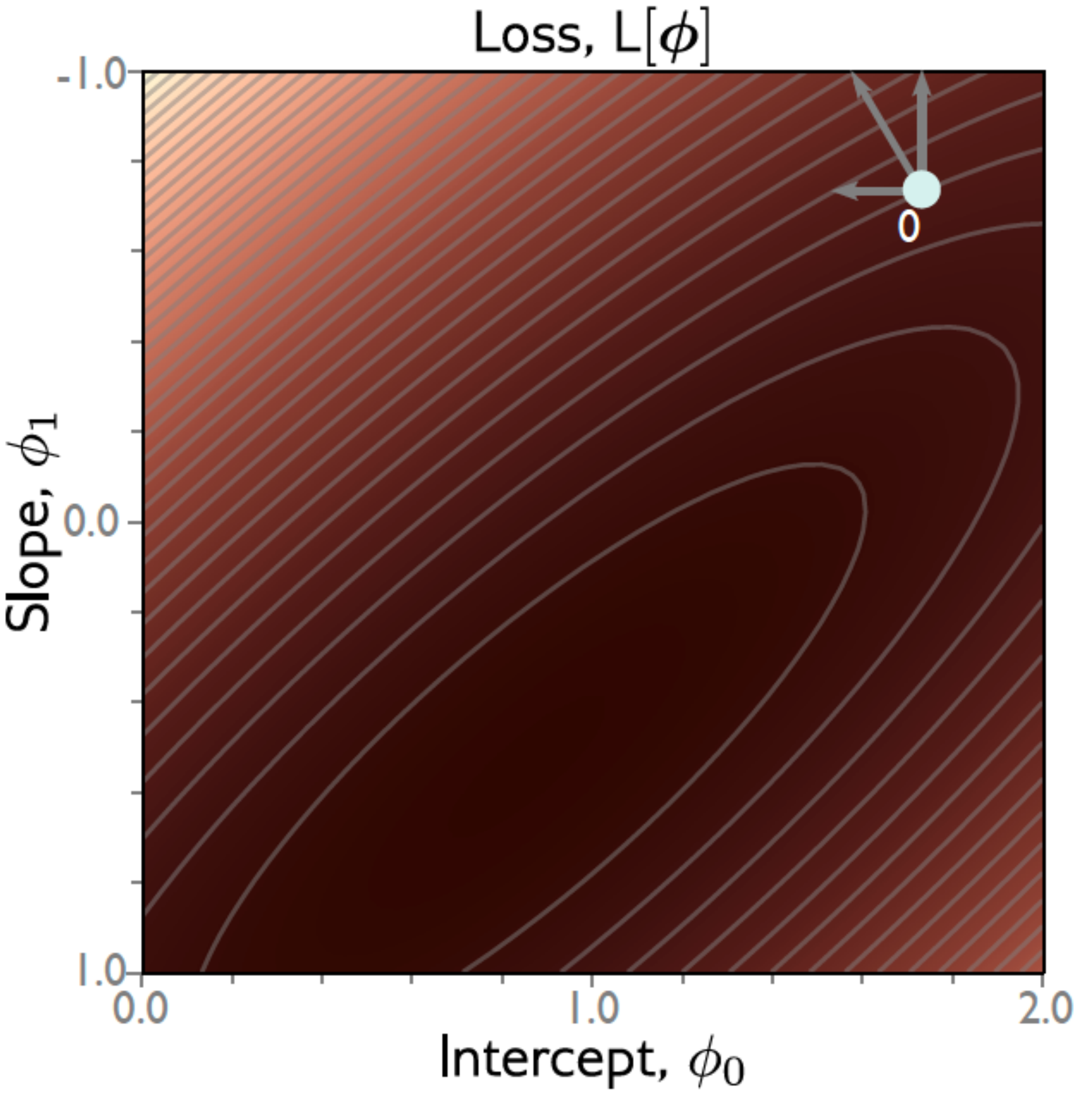
\frac{\partial \ell_i}{\partial \boldsymbol{\phi}} = \begin{bmatrix} \frac{\partial \ell_i}{\partial \phi_0} \\ \frac{\partial \ell_i}{\partial \phi_1} \end{bmatrix} = \begin{bmatrix} 2(\phi_0 + \phi_1 x_i - y_i) \\ 2x_i(\phi_0 + \phi_1 x_i - y_i) \end{bmatrix}
$$

Gradient descent



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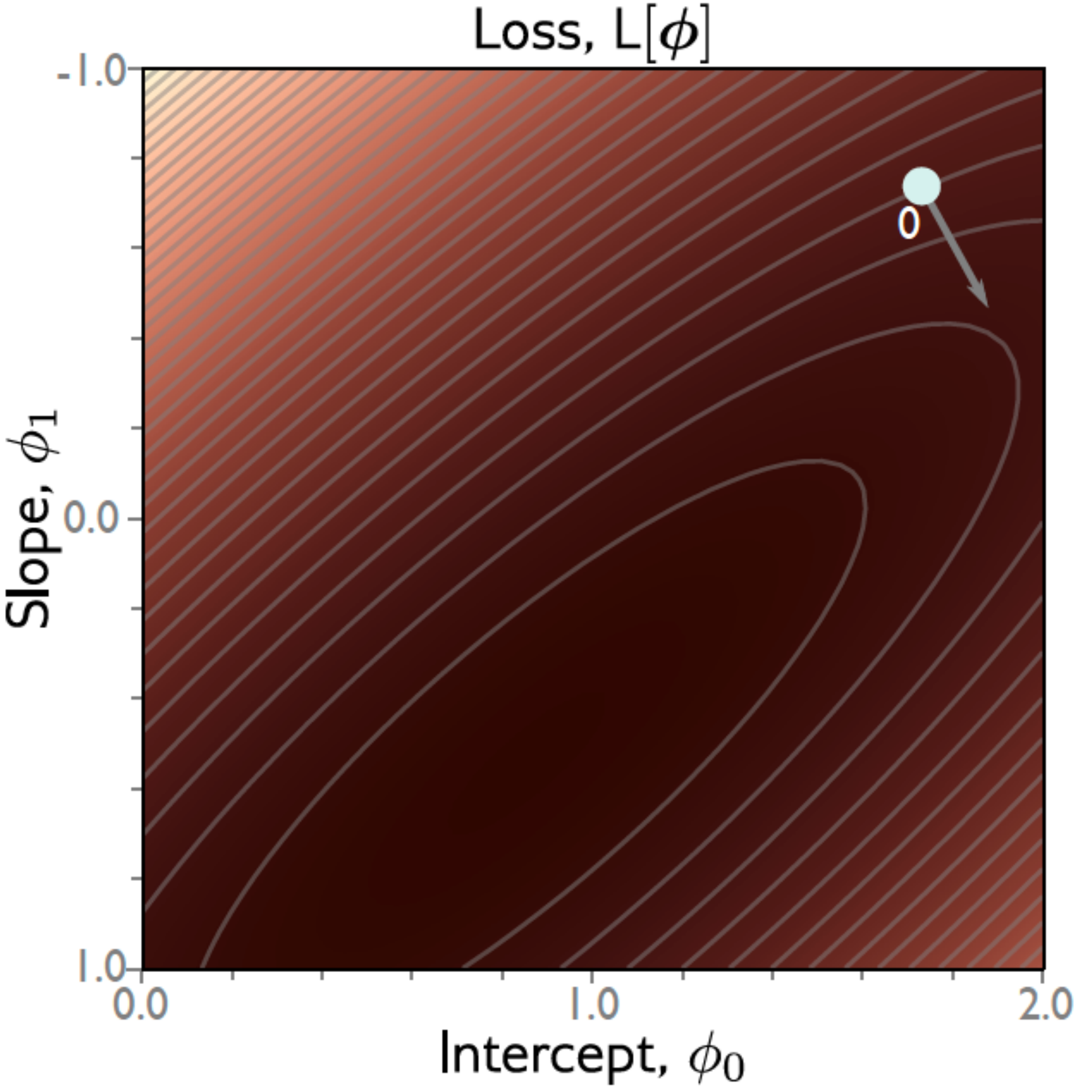

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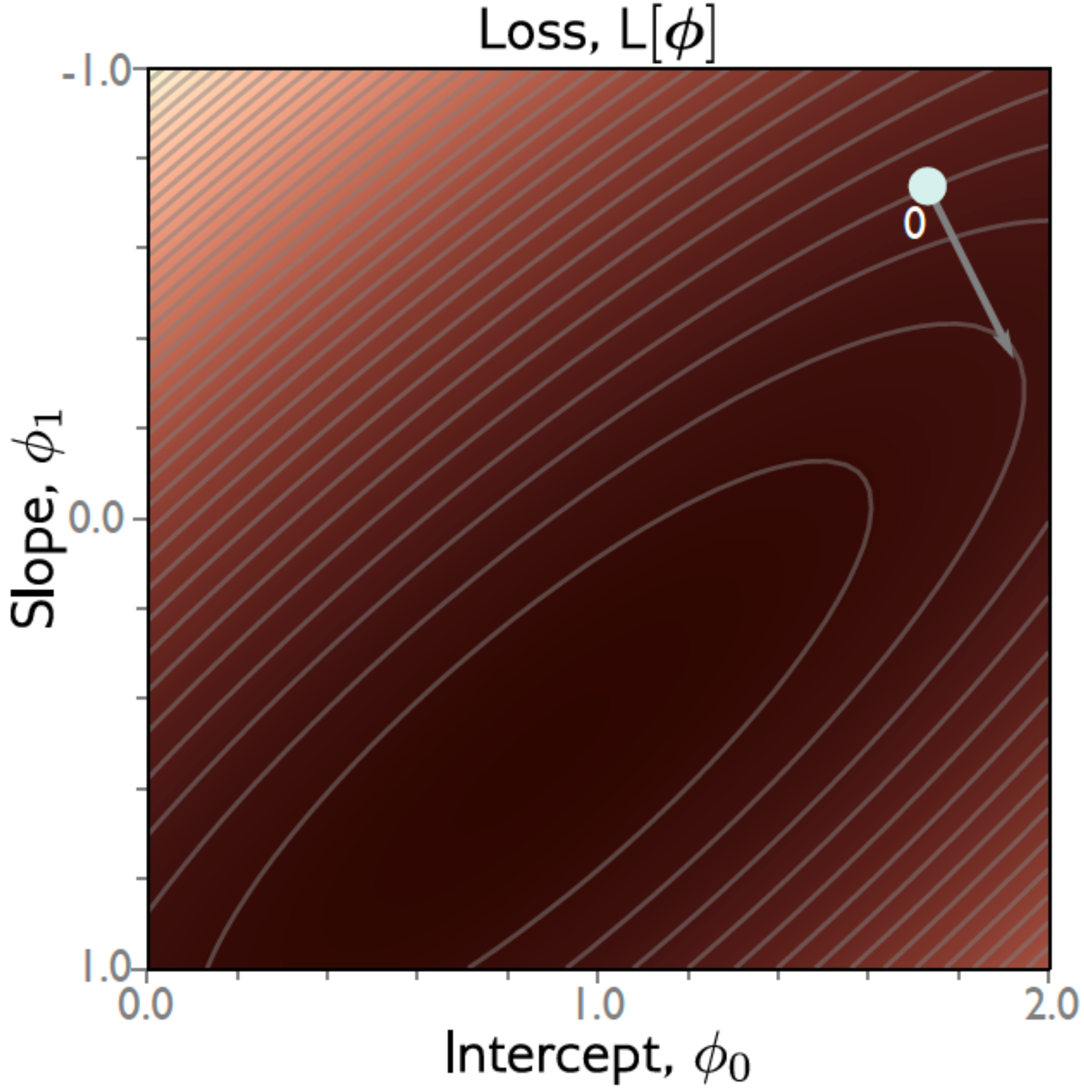
Step 2: Update parameters according to rule

$$\phi \longleftarrow \phi - \alpha \frac{\partial L}{\partial \phi}$$

α = step size or learning rate if fixed

Gradient descent



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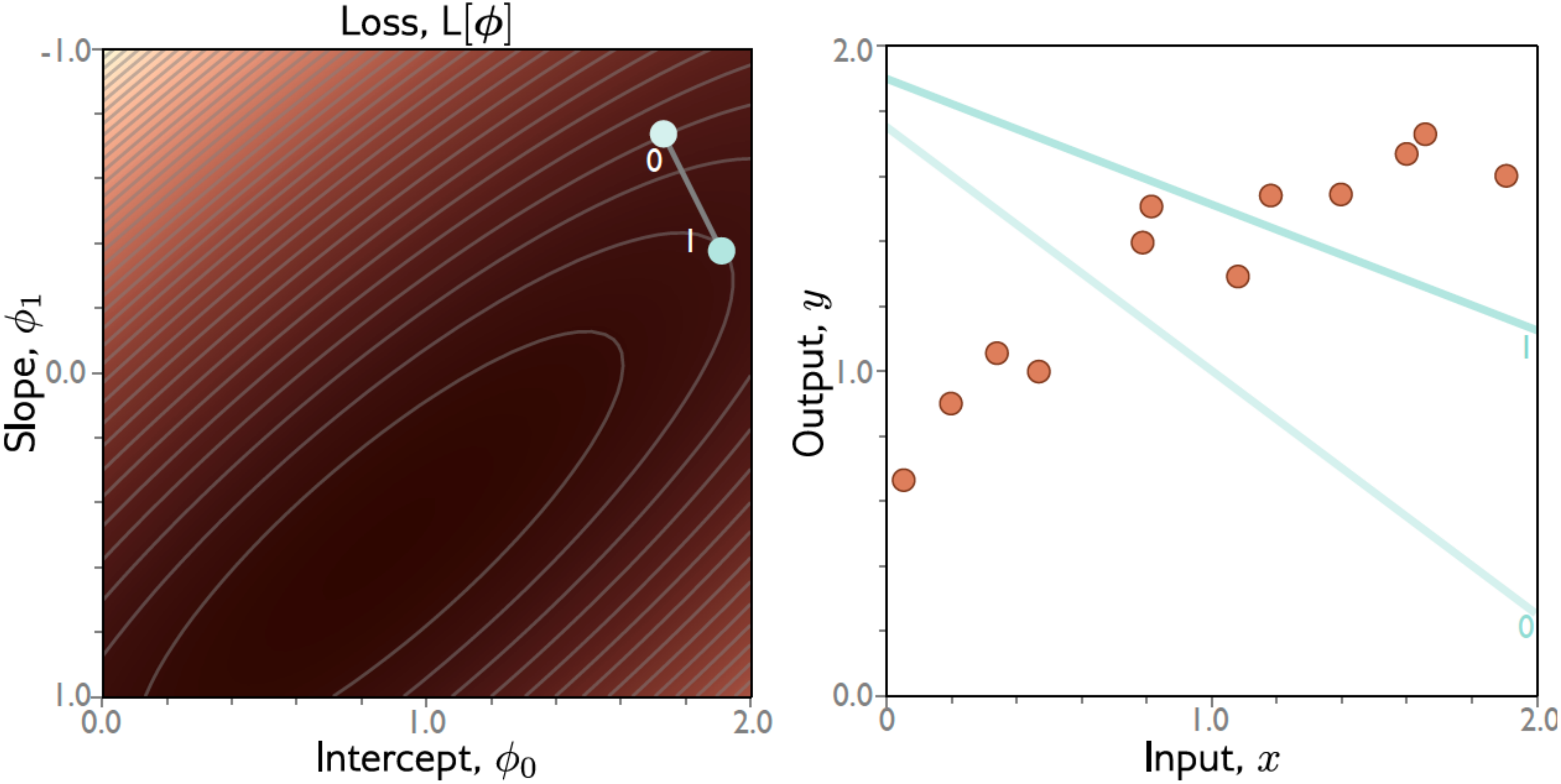
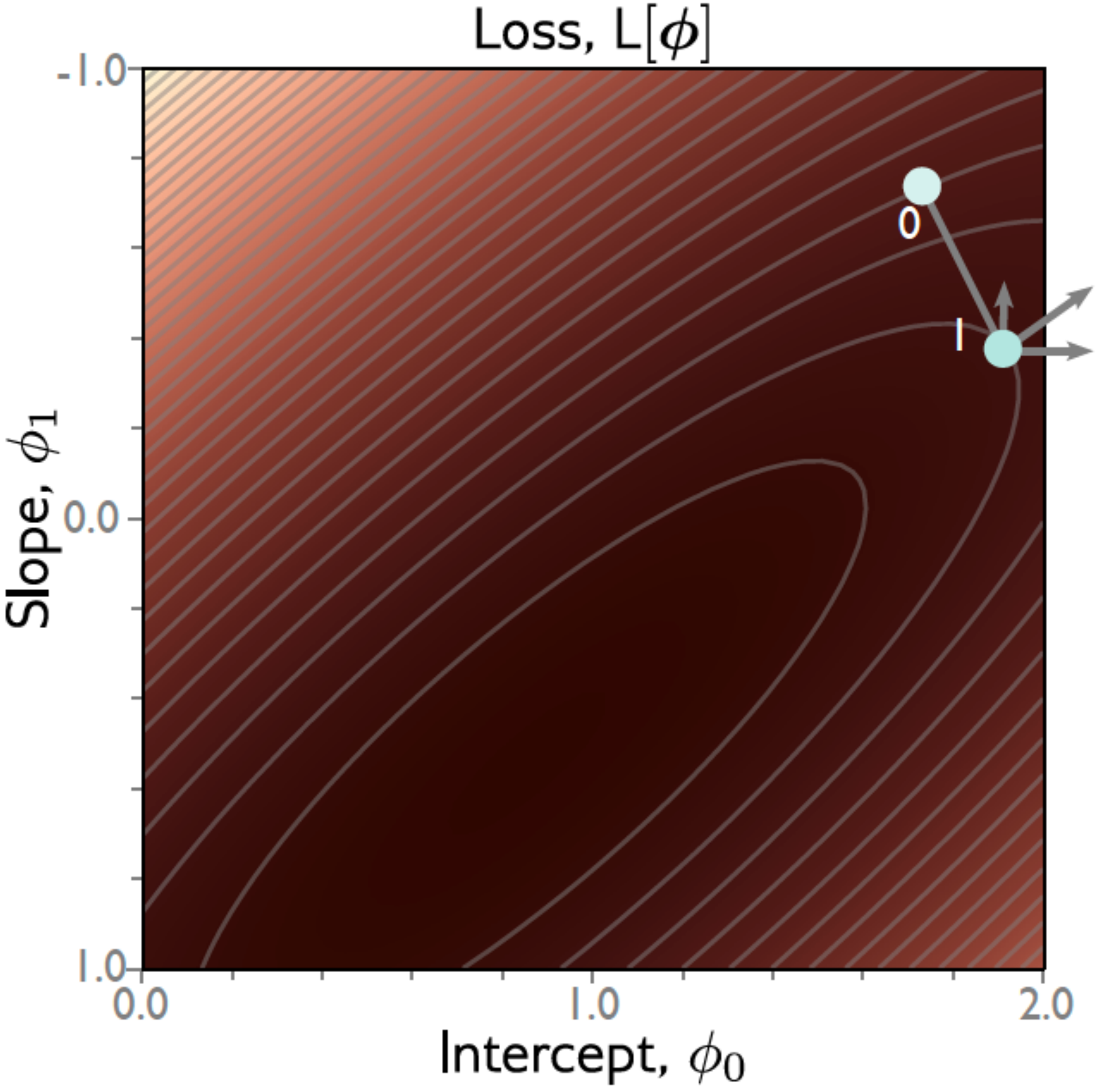
α = step size

Gradient descent



Gradient descent



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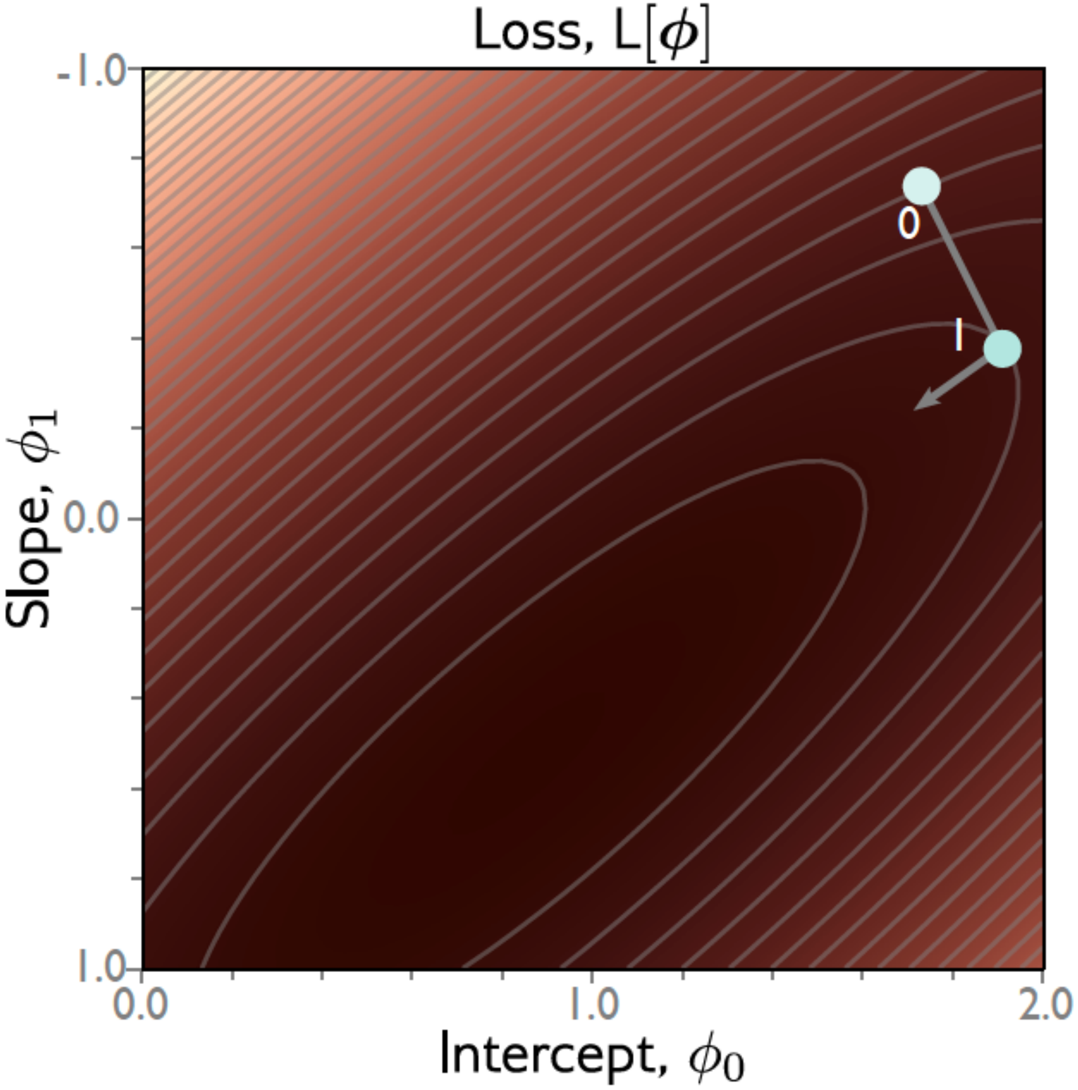

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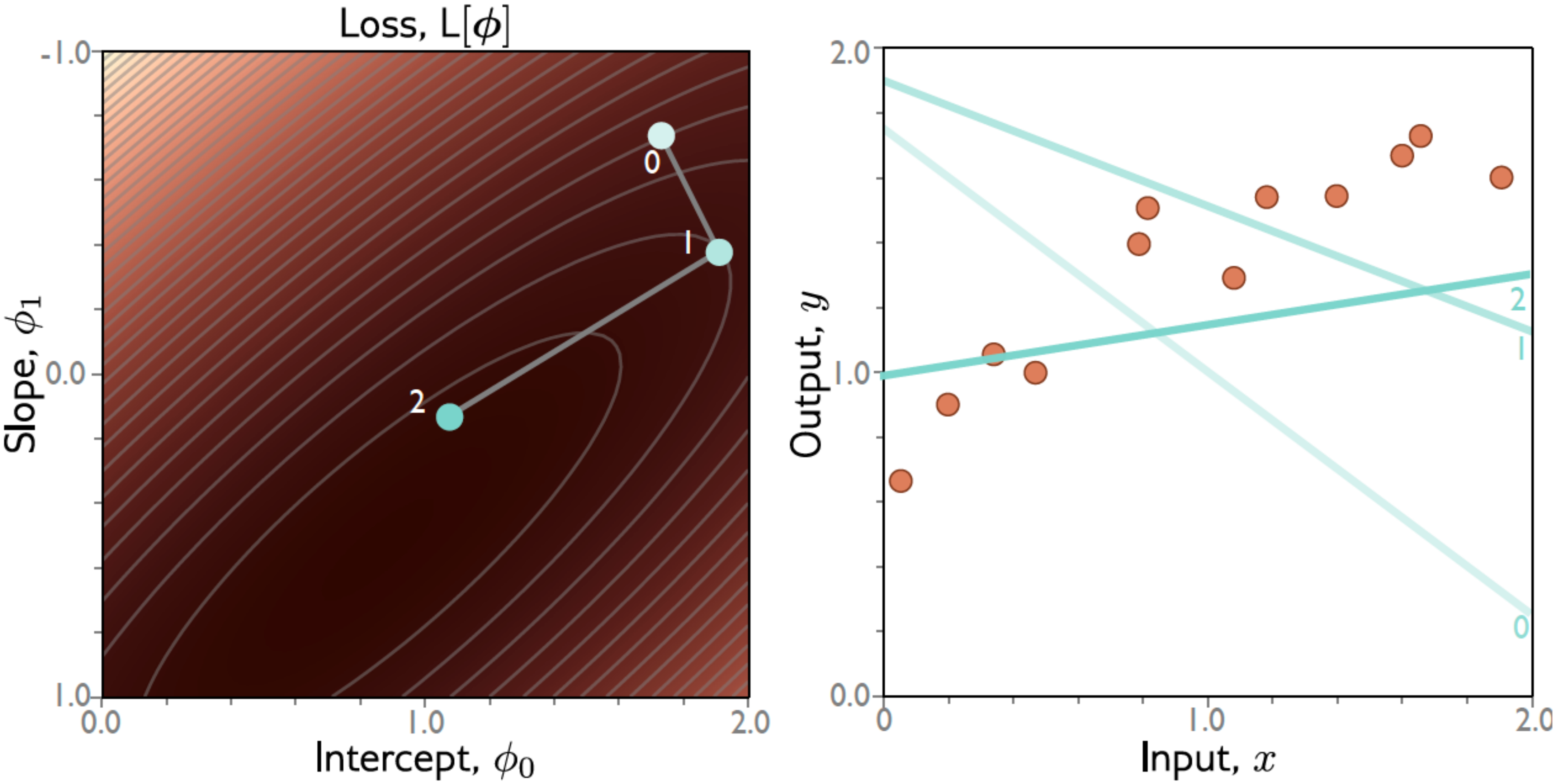
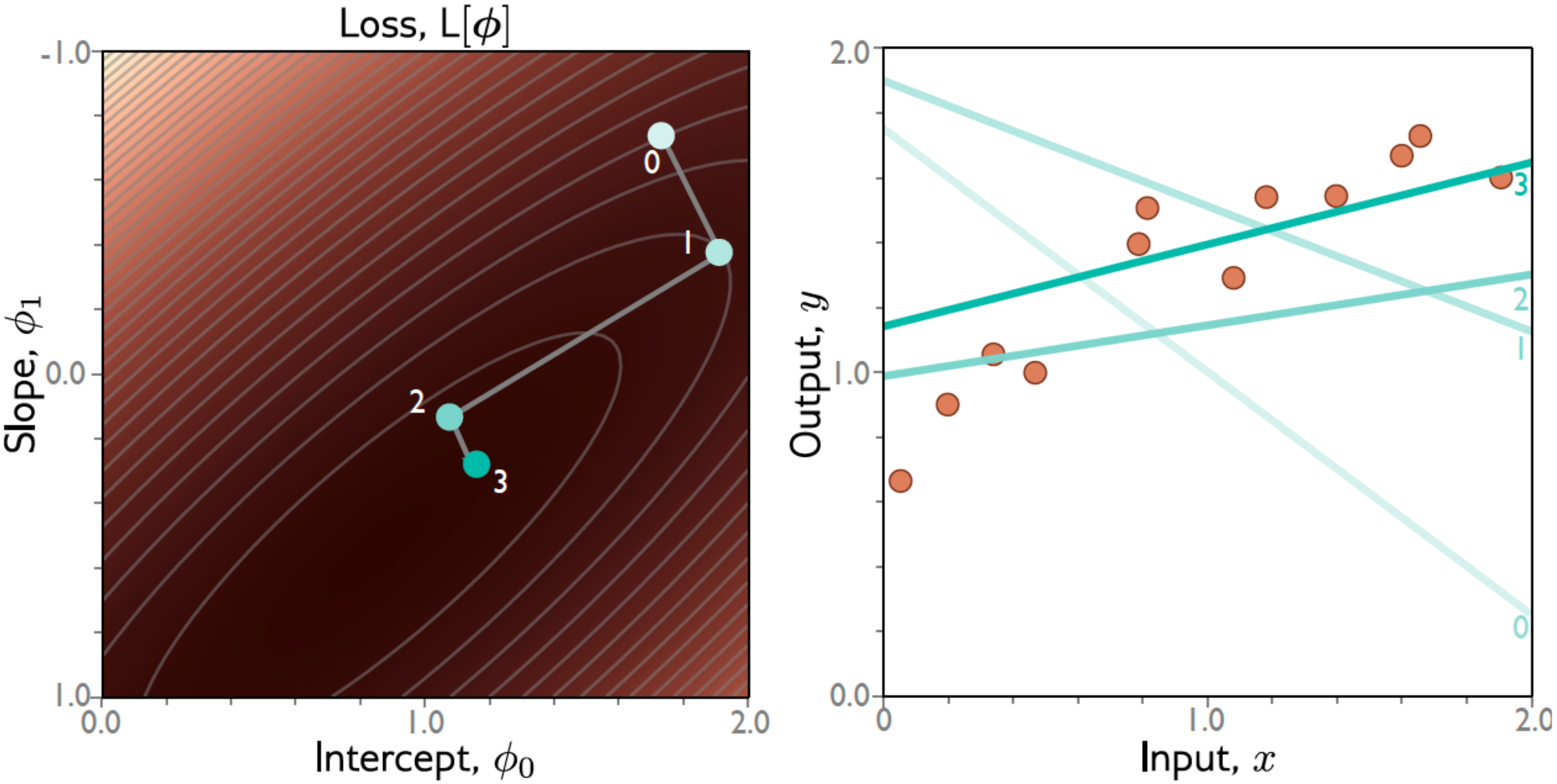


Gradient descent



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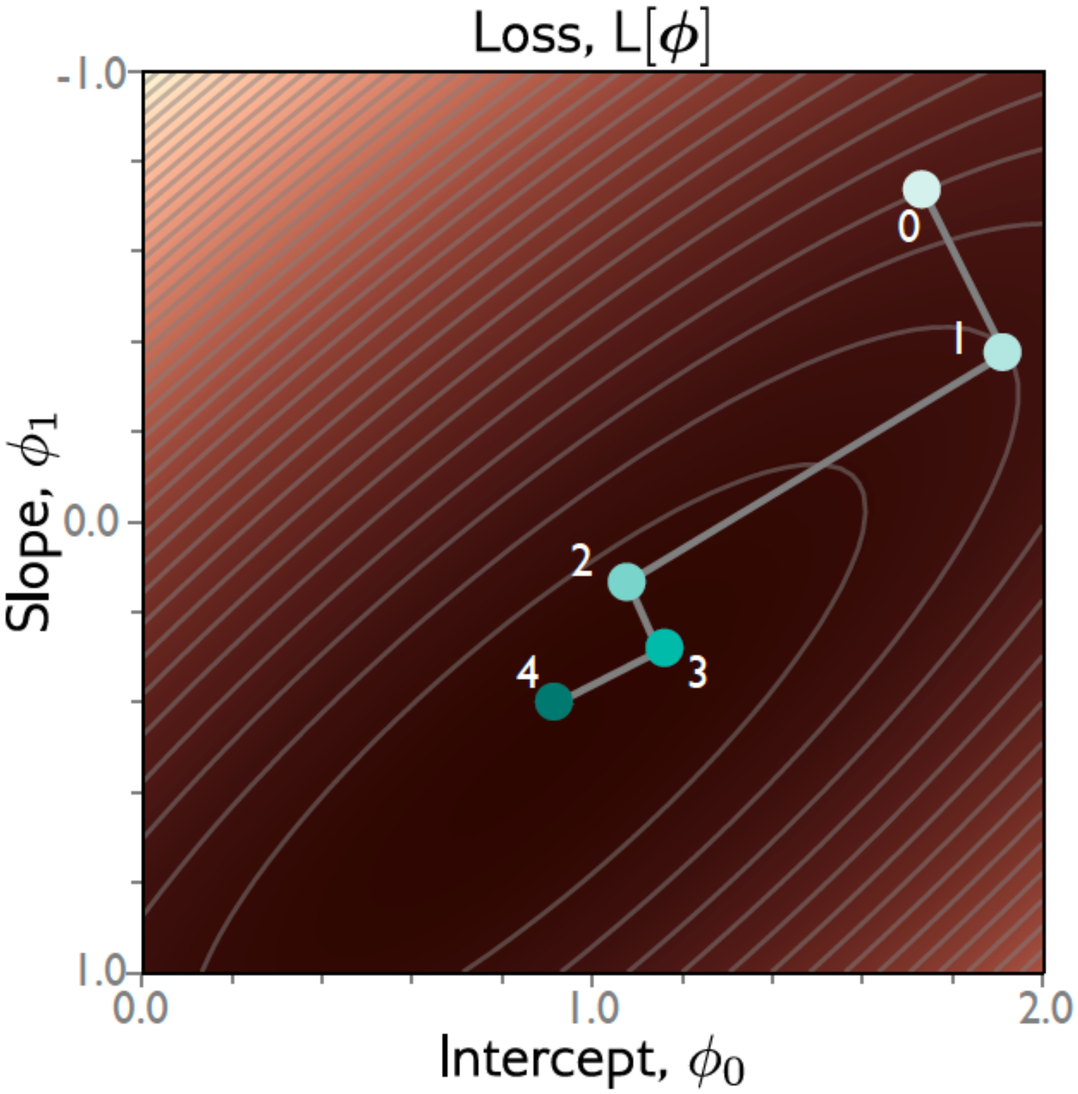
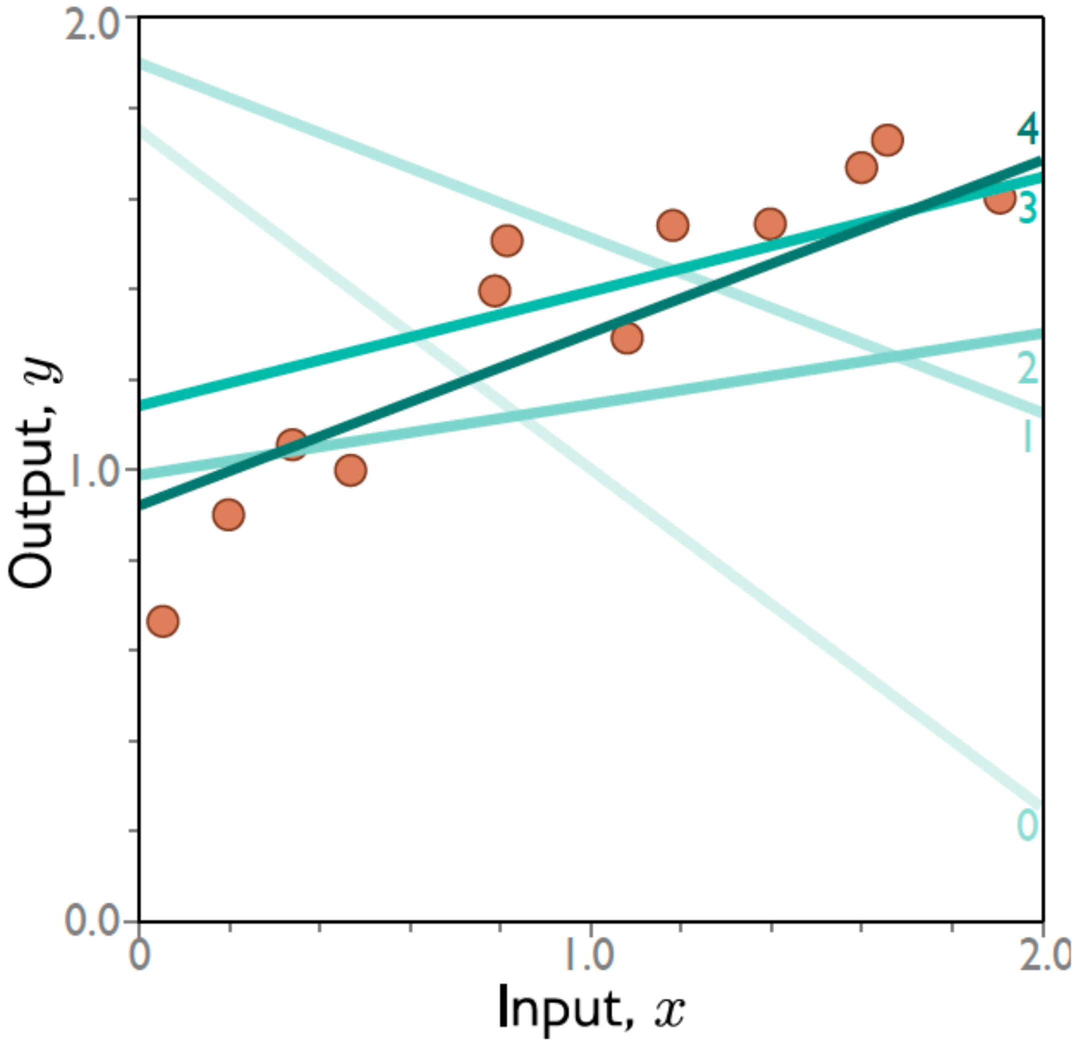
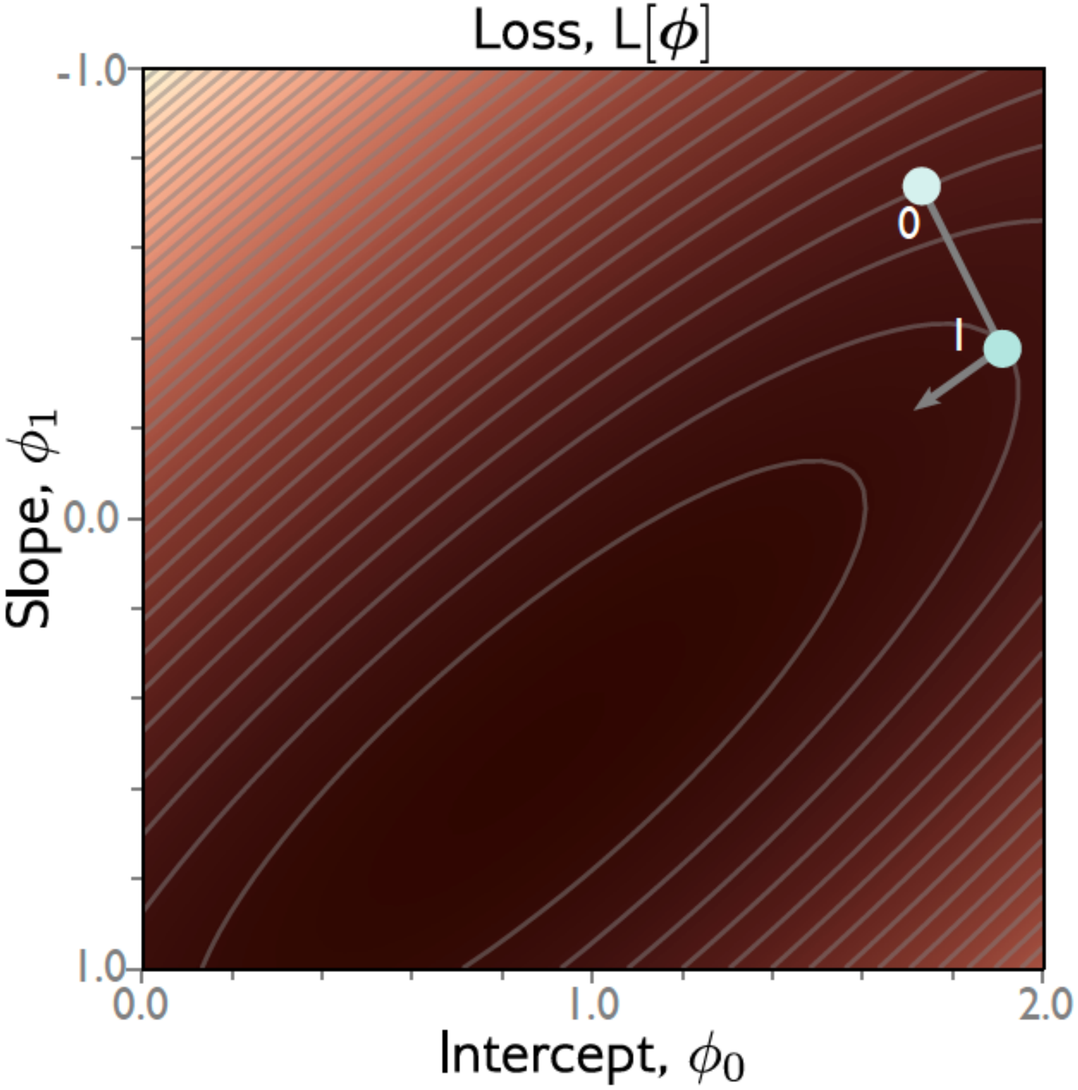




Line Search



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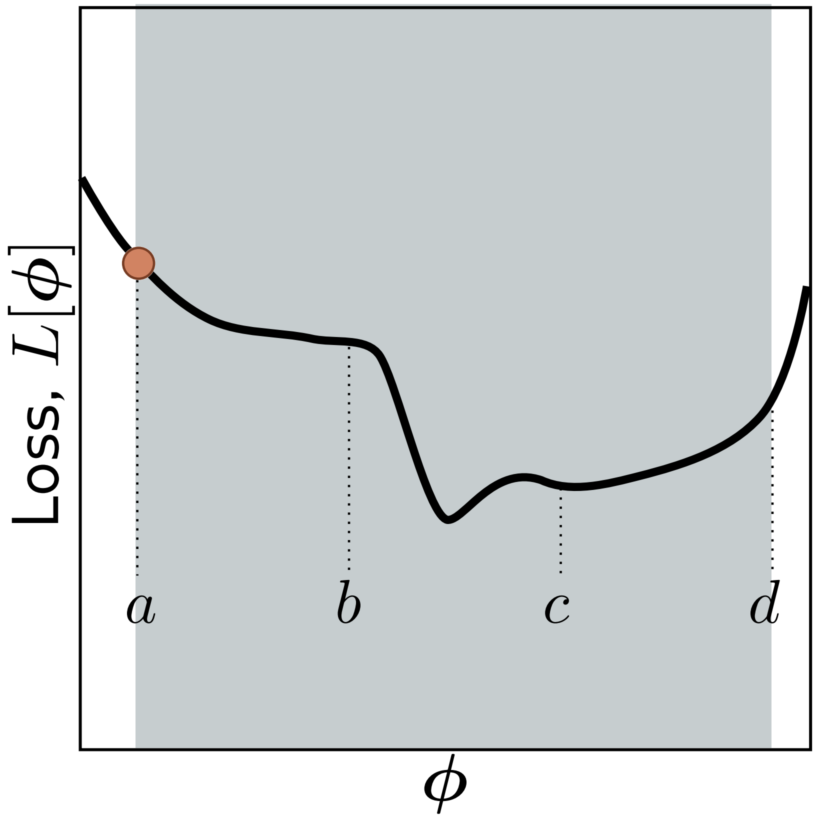
Line Search (bracketing)



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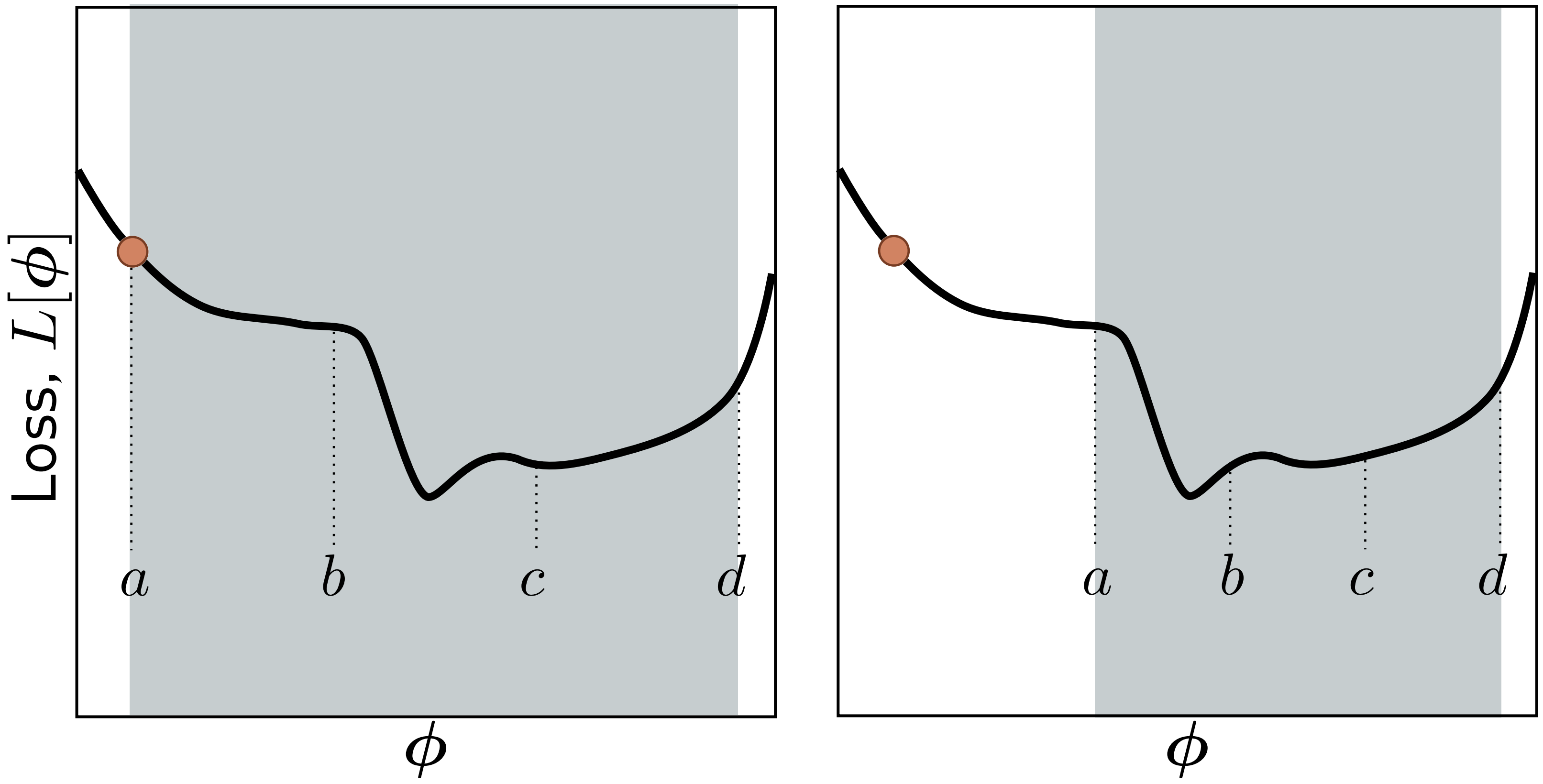

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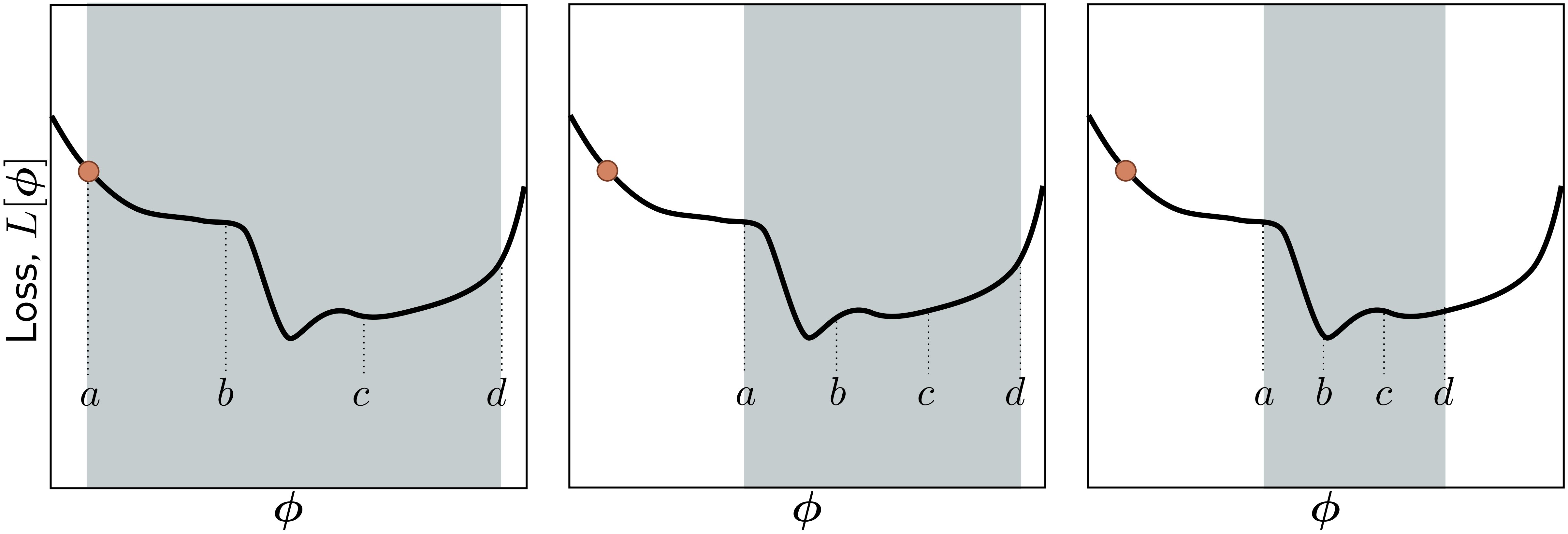
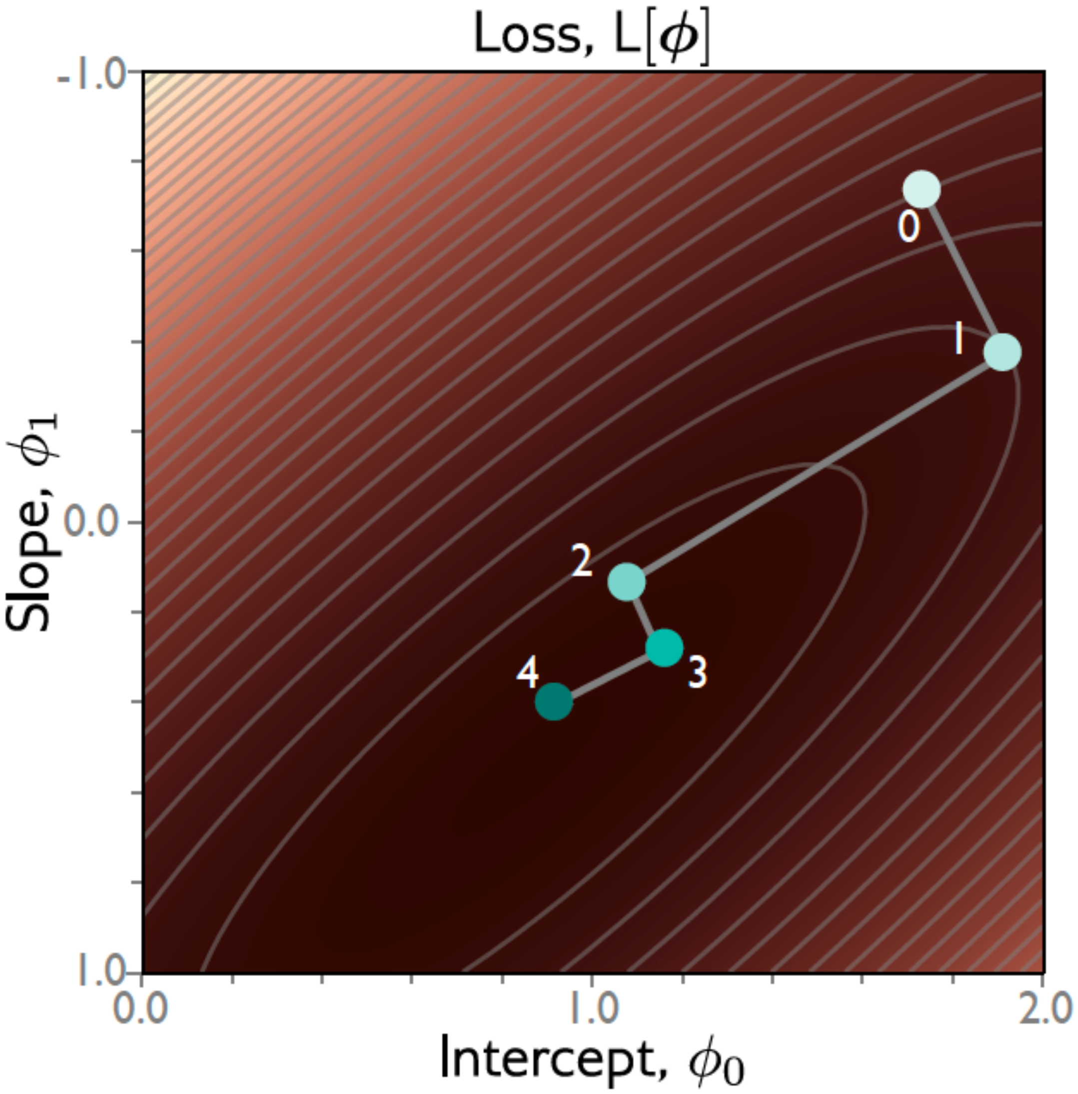
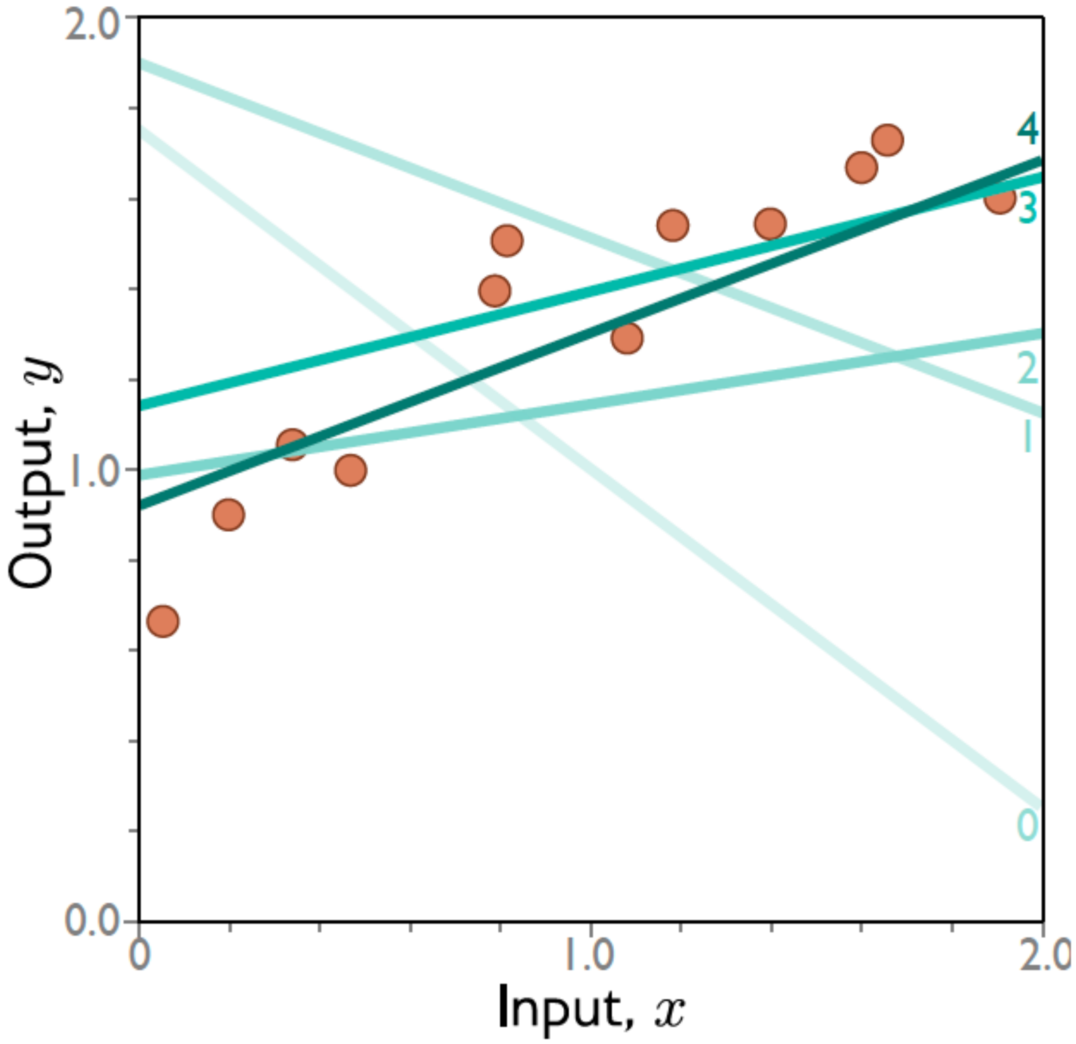
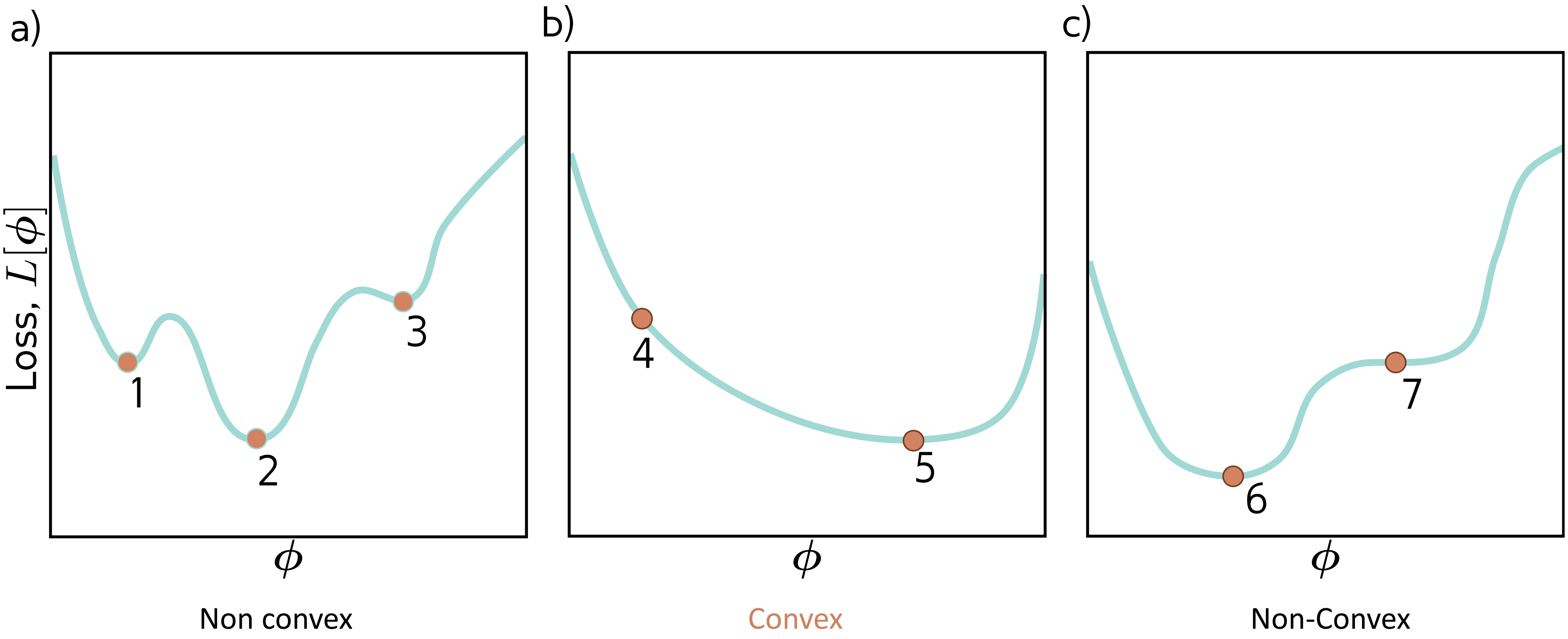


Gradient descent





Convex problems



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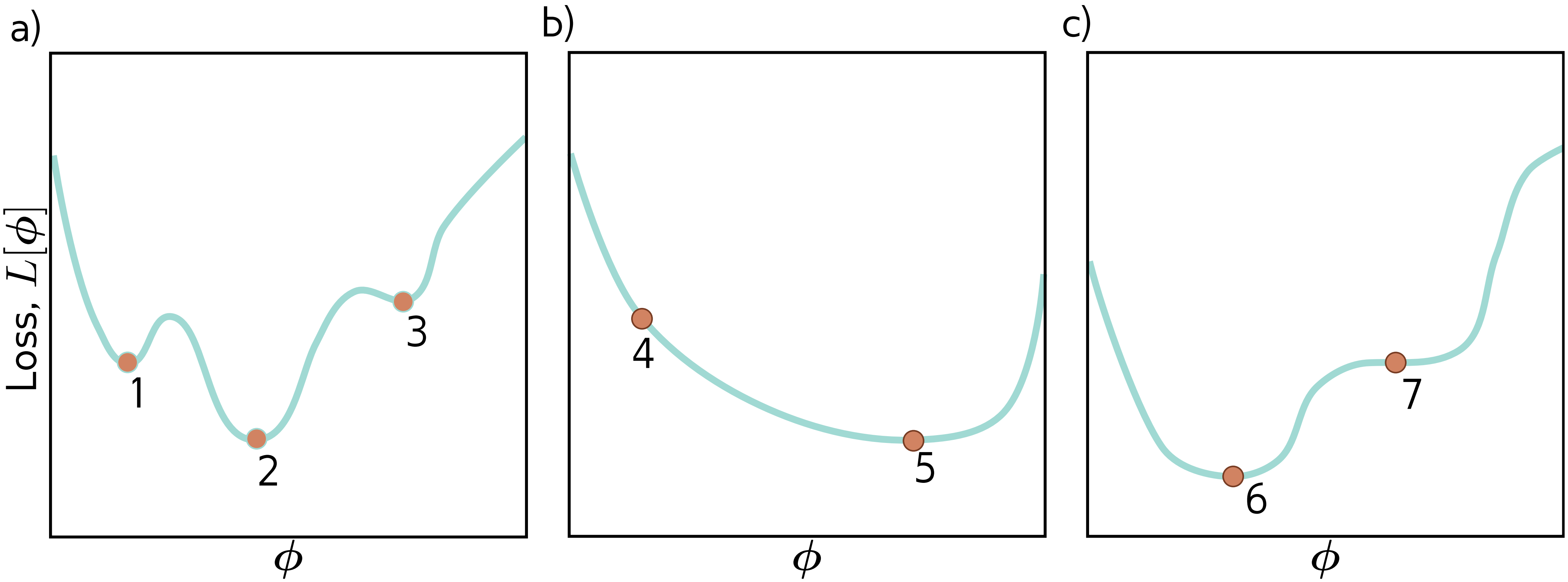


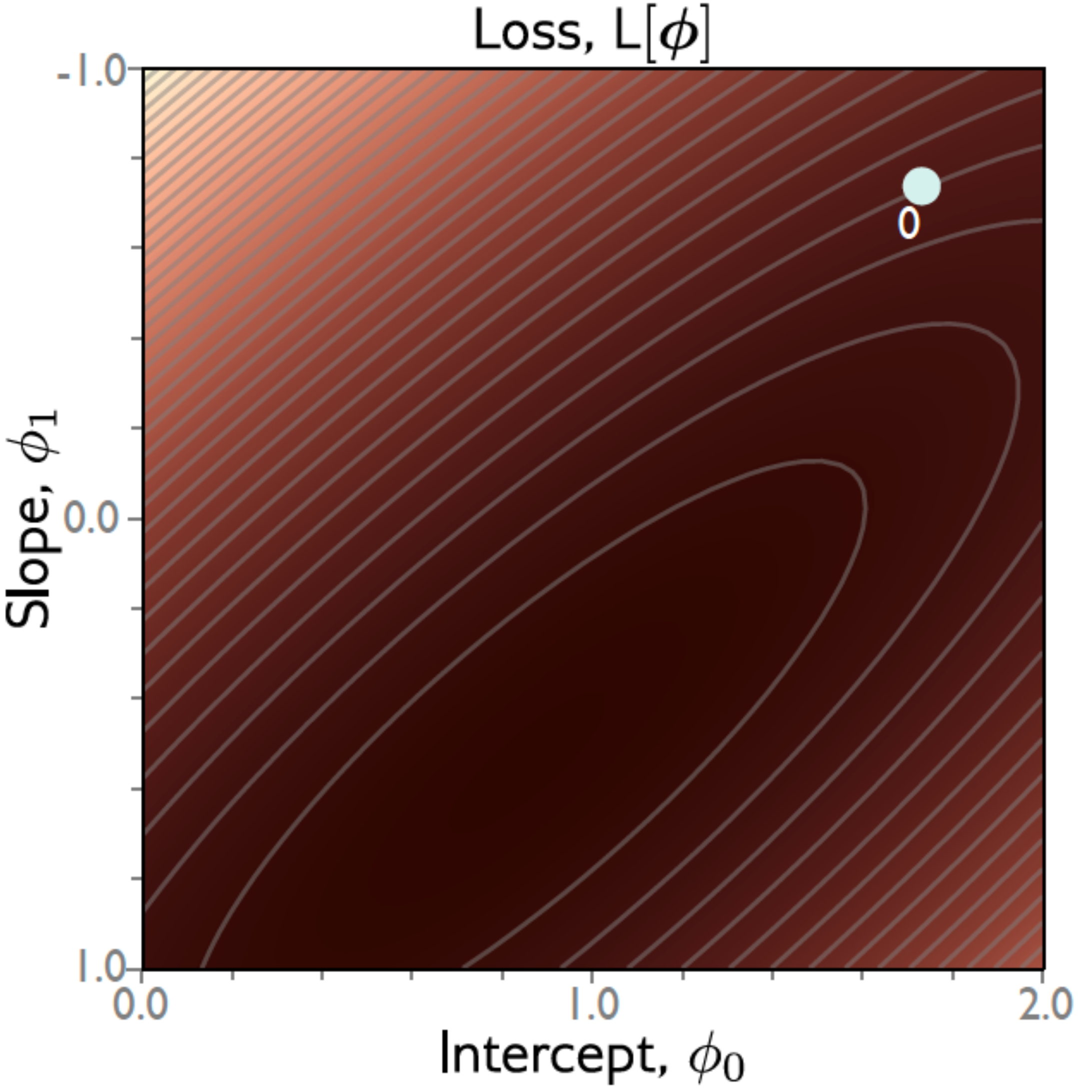
Non convex

Convex

Non-Convex

Test for convexity is that 2nd derivative is positive everywhere

Convexity in higher dimensions



Test for convexity is that determinant of Hessian (2nd derivative matrix) is positive everywhere.

$$\mathbf{H}[\boldsymbol{\phi}] = \begin{bmatrix} \frac{\partial^2 L}{\partial \phi_0^2} & \frac{\partial^2 L}{\partial \phi_0 \partial \phi_1} \\ \frac{\partial^2 L}{\partial \phi_1 \partial \phi_0} & \frac{\partial^2 L}{\partial \phi_1^2} \end{bmatrix}$$

$$\mathbf{H}[\boldsymbol{\phi}] = \frac{\partial^2 L}{\partial \phi_0^2}\frac{\partial^2 L}{\partial \phi_1^2} - \frac{\partial^2 L}{\partial \phi_0 \partial \phi_1}\frac{\partial^2 L}{\partial \phi_1 \partial \phi_0}$$

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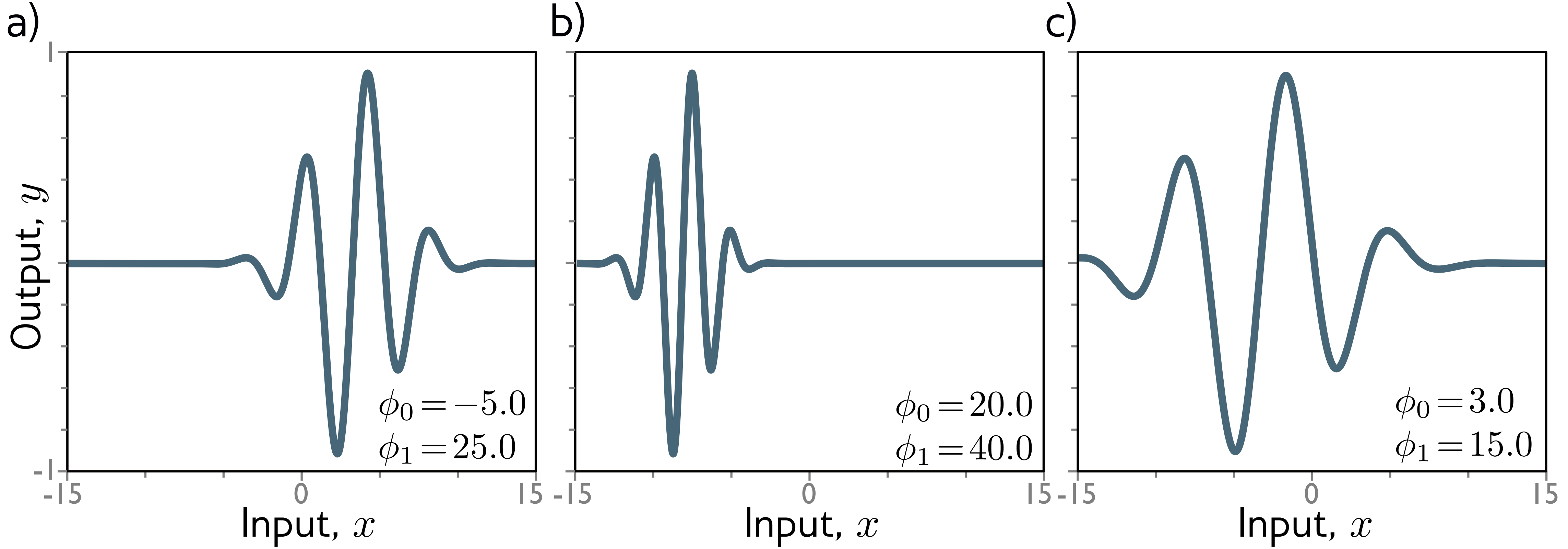
Gabor model

$$\mathrm{f}[x, \boldsymbol{\phi}] = \sin[\phi_0 + 0.06 \cdot \phi_1 x] \cdot \exp\left(-\frac{(\phi_0 + 0.06 \cdot \phi_1 x)^2}{8.0}\right)$$



Gabor model

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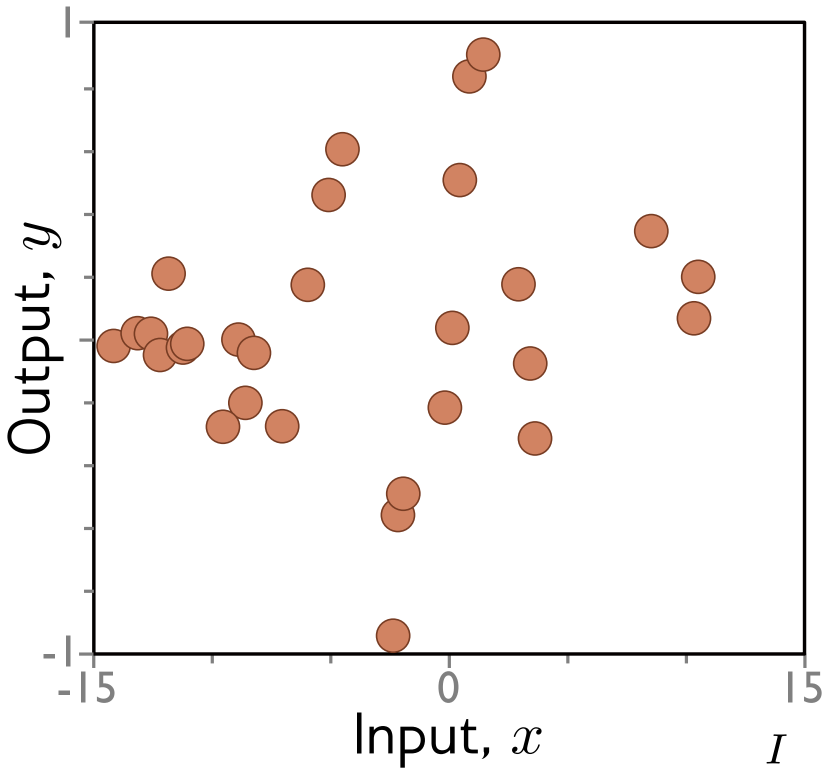
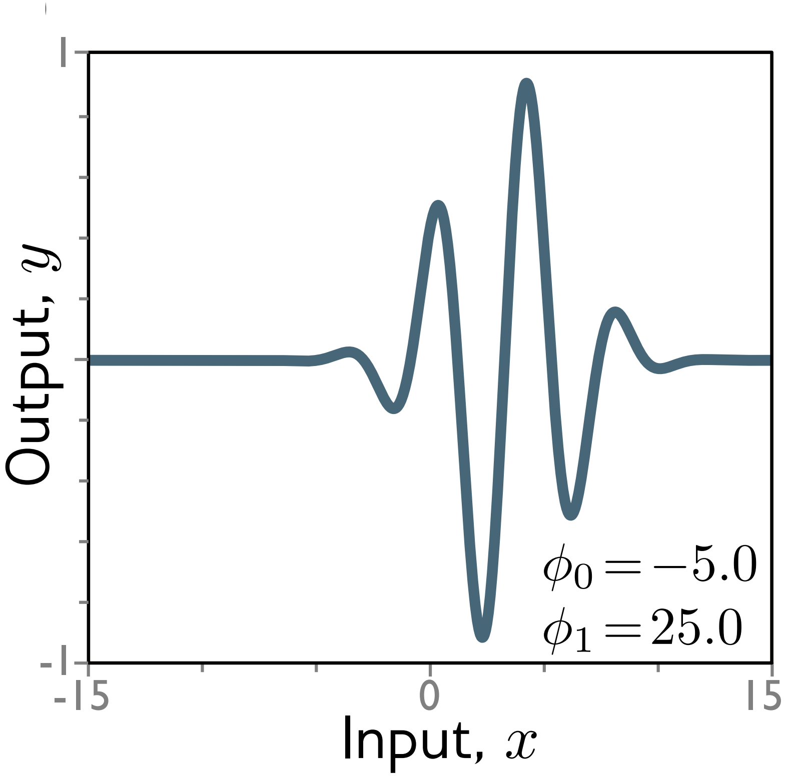
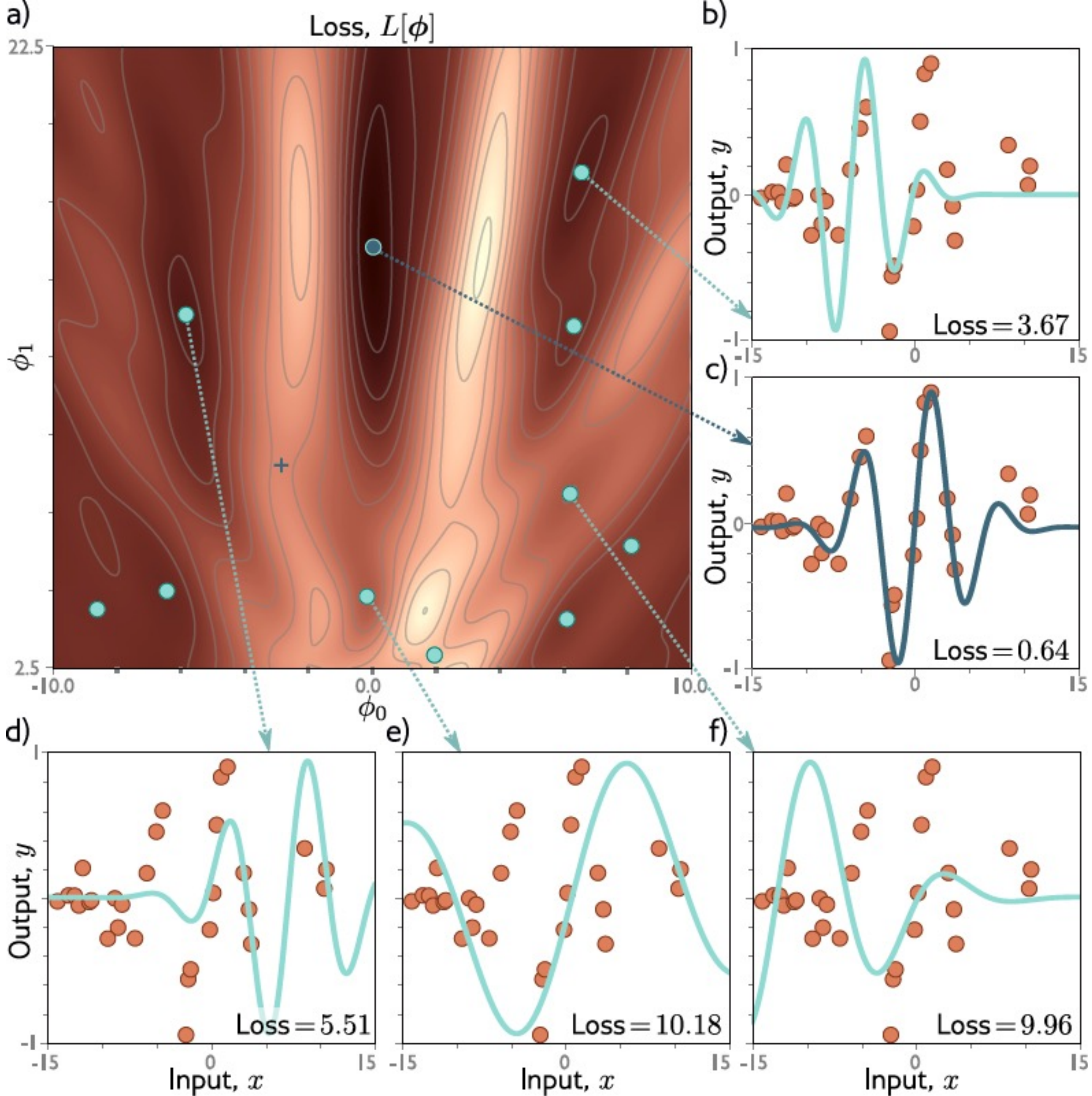
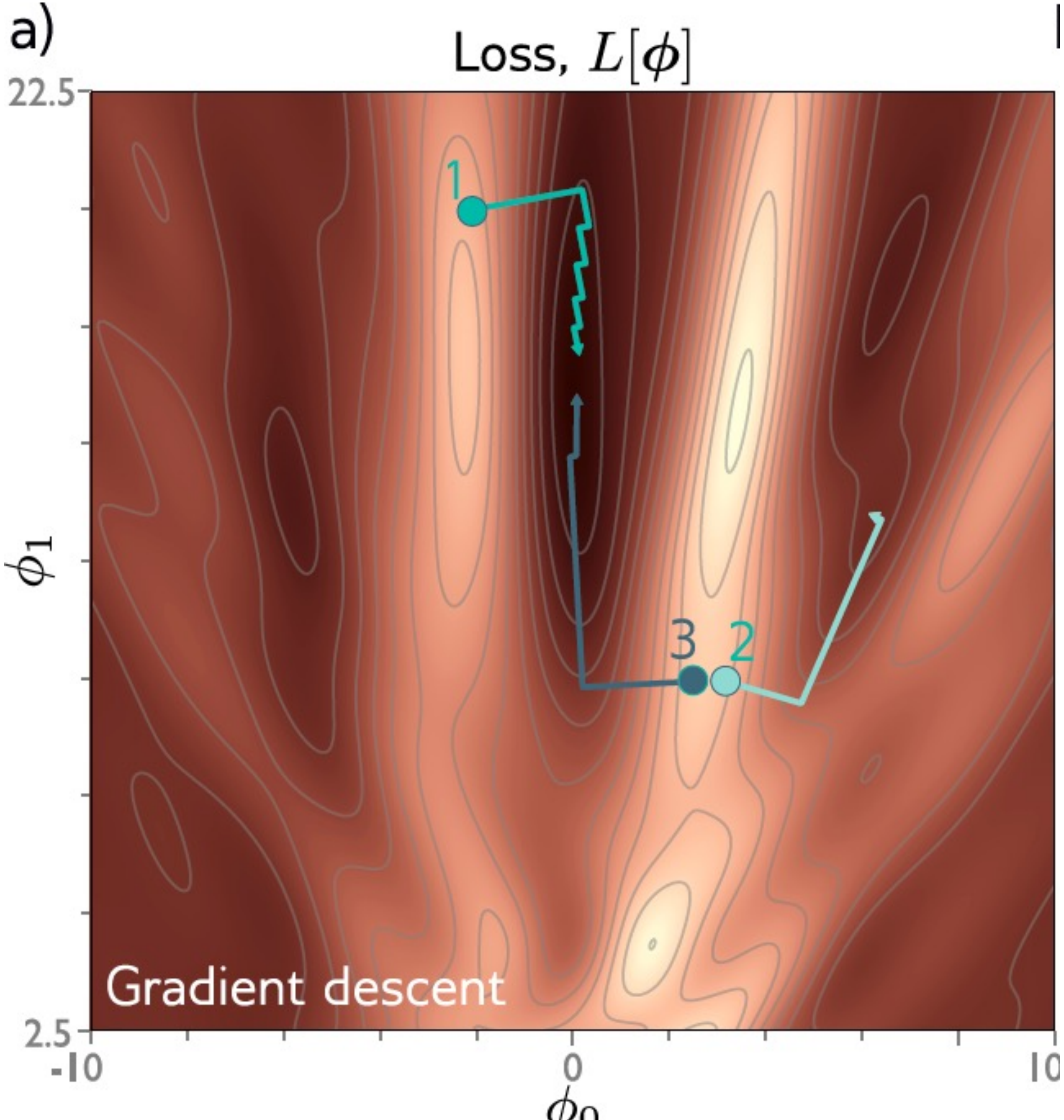




$$L[\boldsymbol{\phi}] = \sum_{i=1}^{I} (\mathrm{f}[x_i, \boldsymbol{\phi}] - y_i)^2$$



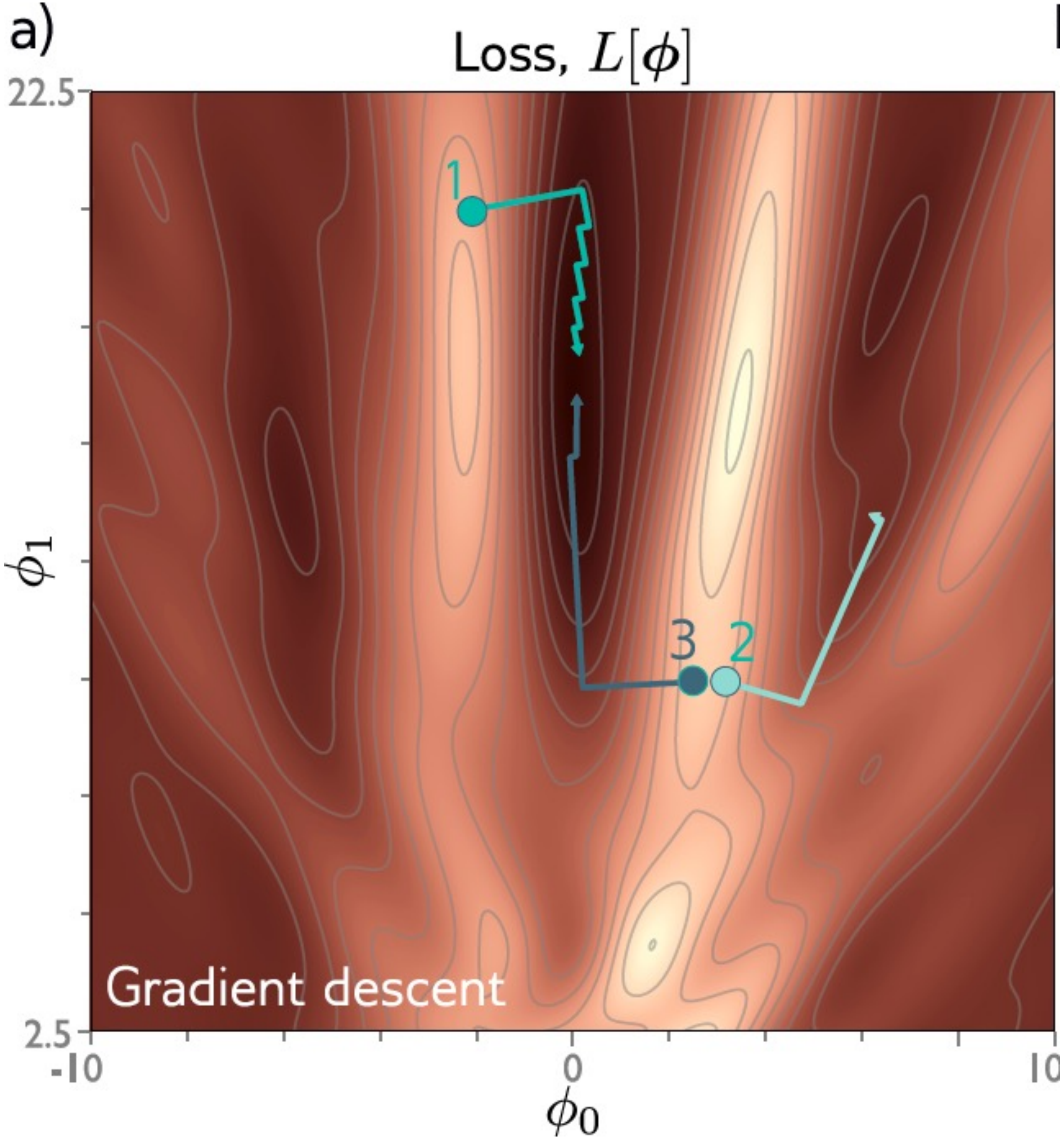
a)
Loss, $L[\phi]$
22.5
2.5
ϕ_1
-10.0
0.0
10.0
ϕ_0
b)
Output, y
Loss = 3.67
c)
Output, y
Loss = 0.64
d)
Output, y
Input, x
Loss = 5.51
e)
Input, x
Loss = 10.18
f)
Input, x
Loss = 9.96
1
0
-1
-15
0
15



- Gradient descent gets to the global minimum if we start in the right "valley"
- Otherwise, descent to a local minimum
- Or get stuck near a saddle point

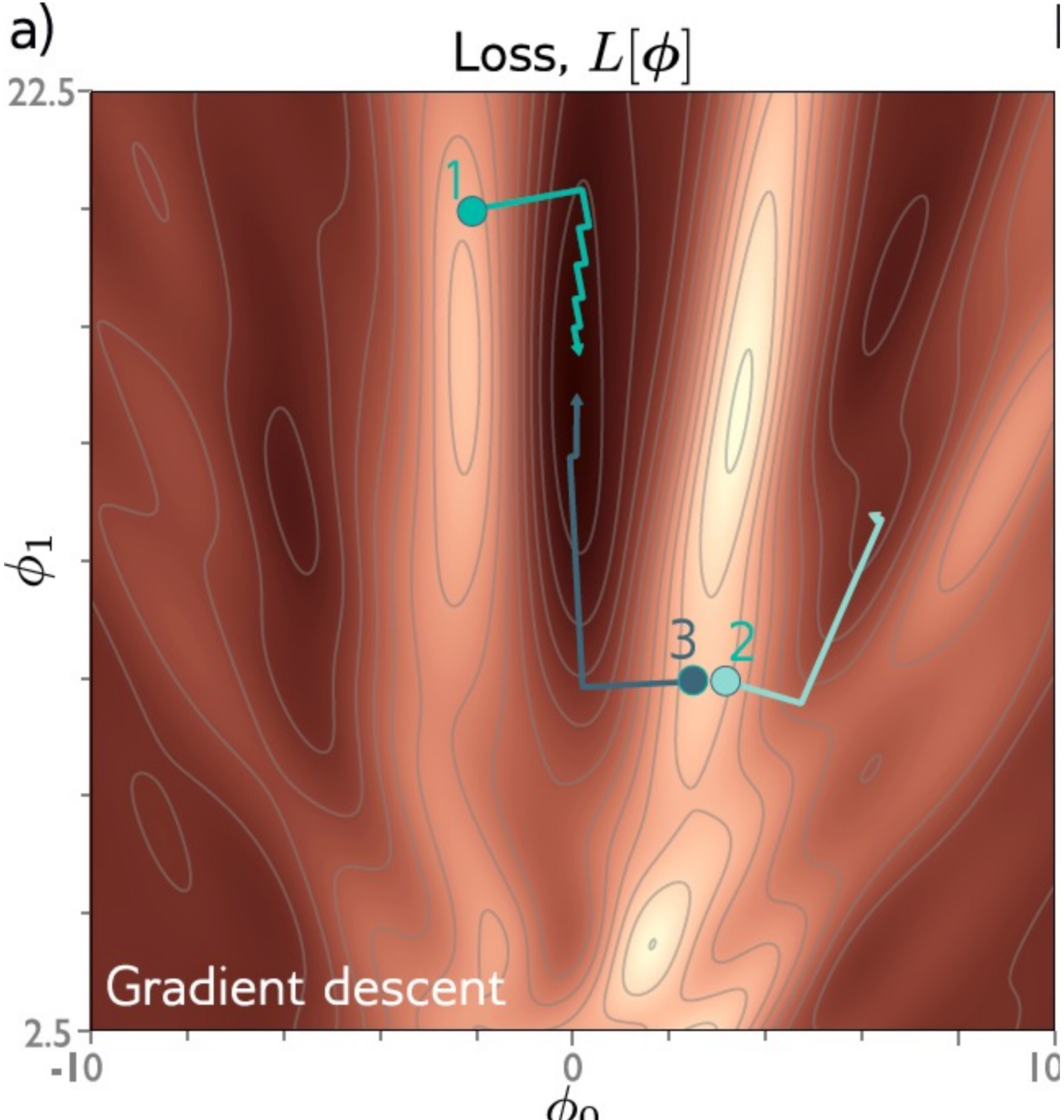
Fitting models

- Maths overview
- Gradient descent algorithm
- Linear regression example
- Gabor model example
- Stochastic gradient descent
- Momentum
- Adam



IDEA: add noise

- Stochastic gradient descent
- Compute gradient based on only a subset of points – a mini-batch
- Work through dataset sampling without replacement
- One pass though the data is called an epoch



Stochastic gradient descent

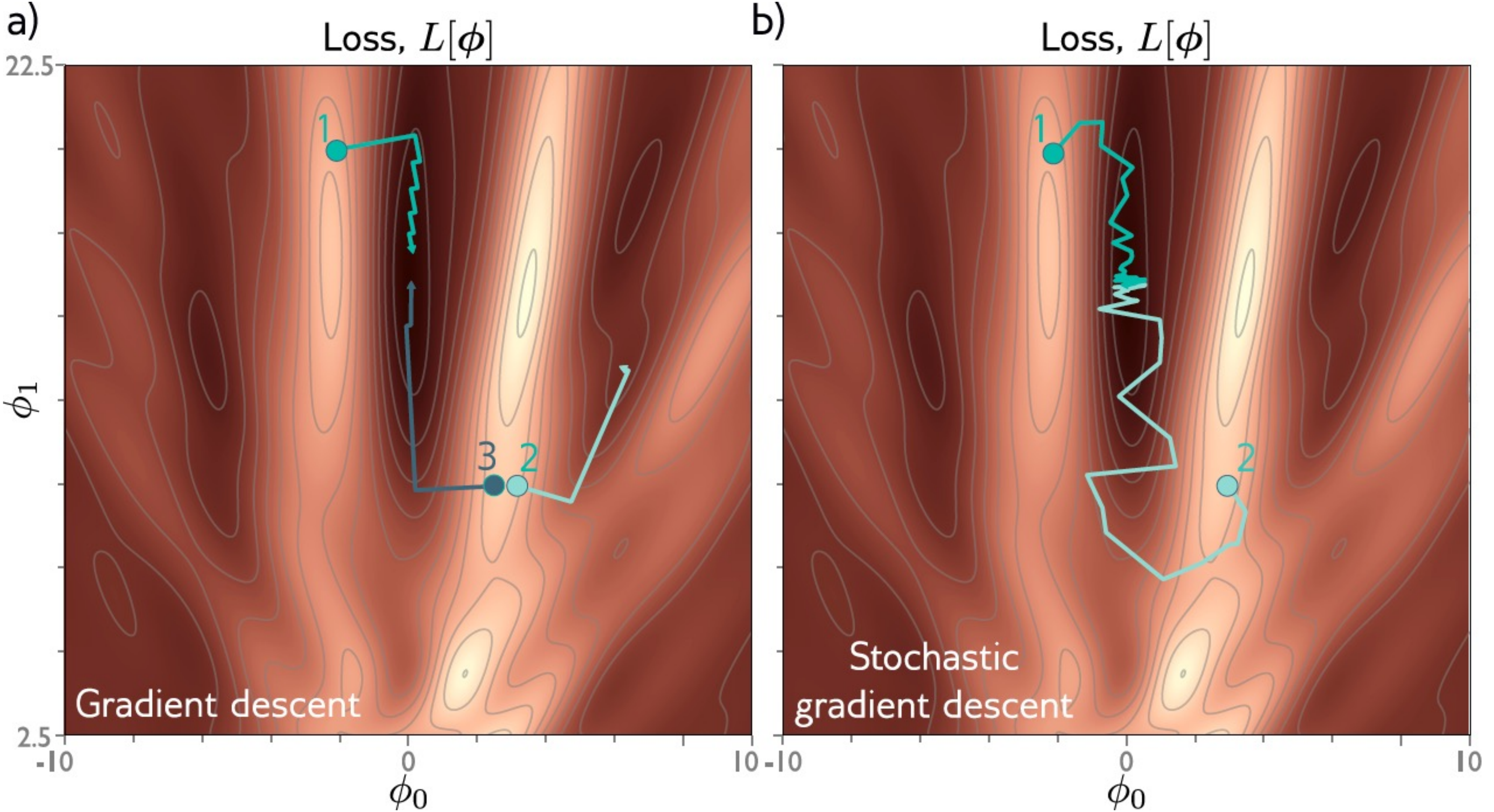
Before (full batch descent)

$$\phi_{t+1} \longleftarrow \phi_t - \alpha \sum_{i=1}^{I} \frac{\partial \ell_i[\phi_t]}{\partial \phi},$$

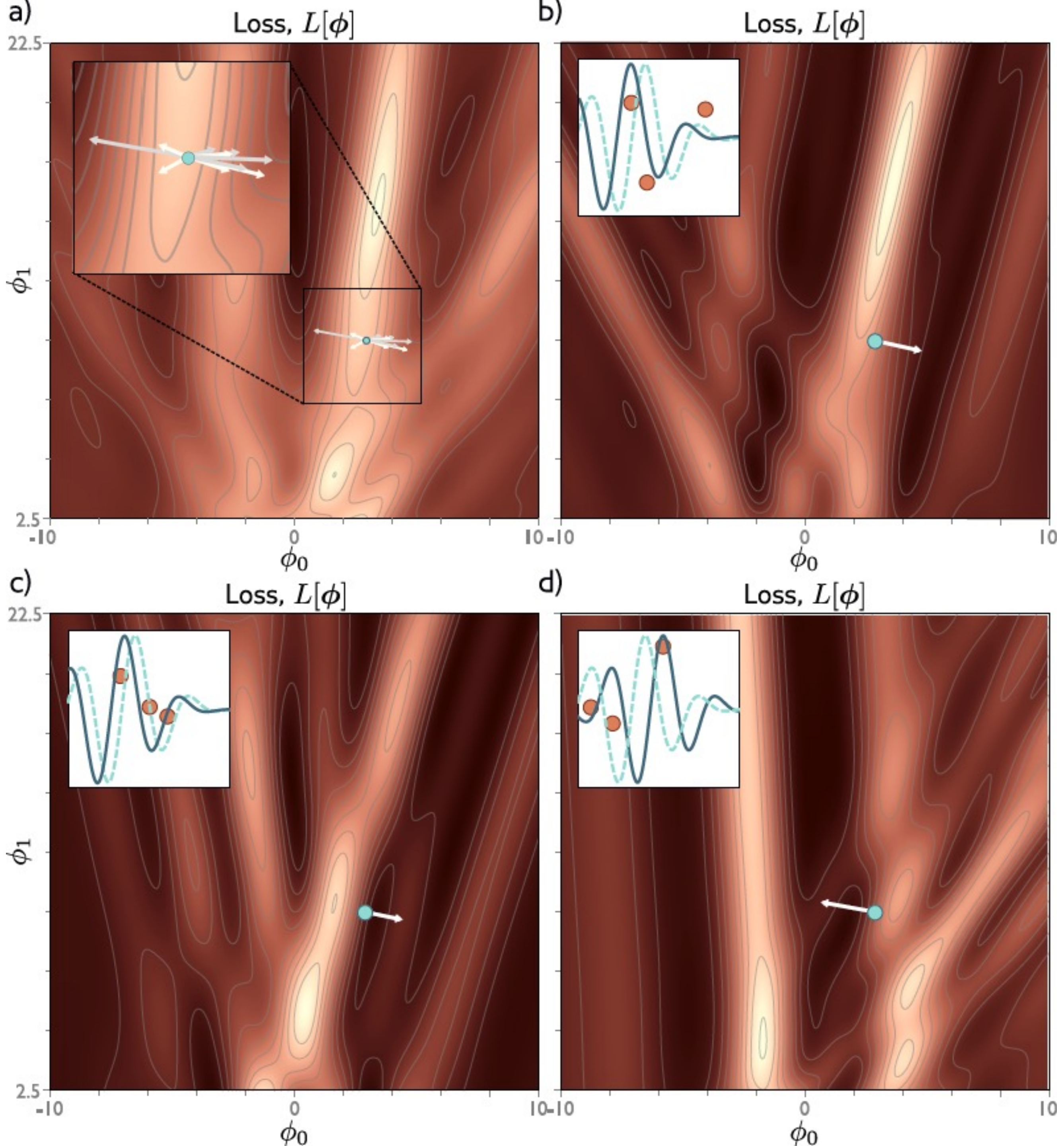
After (SGD)

$$\phi_{t+1} \longleftarrow \phi_t - \alpha \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\phi_t]}{\partial \phi},$$

Fixed learning rate α



a)
Loss, $L[\phi]$
22.5
2.5
ϕ_1
1
2
3
Gradient descent
-10
0
10
ϕ_0
b)
Loss, $L[\phi]$
1
2
Stochastic
gradient descent
-10
0
10
ϕ_0



a)
Loss, $L[\phi]$
b)
Loss, $L[\phi]$
c)
Loss, $L[\phi]$
d)
Loss, $L[\phi]$
22.5
2.5
ϕ_1
ϕ_0
-10
0
10

Properties of SGD

- Can escape from local minima
- Adds noise, but still sensible updates as based on part of data
- Uses all data equally
- Less computationally expensive
- Seems to find better solutions

- Doesn’t converge in traditional sense
- Learning rate schedule – decrease learning rate over time

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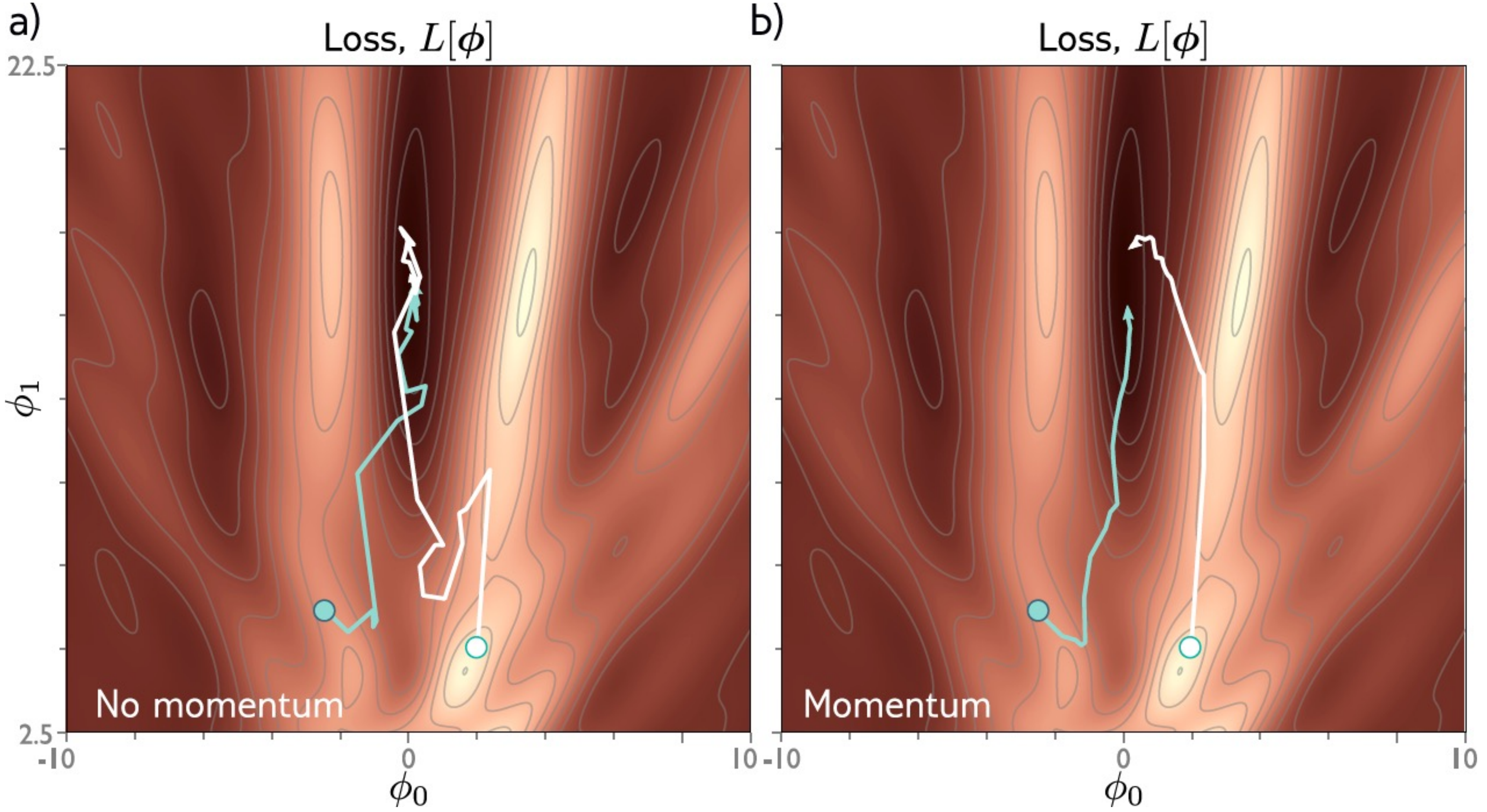
Momentum

- Weighted sum of this gradient and previous gradient

$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta)\sum_{i\in\mathcal{B}_t}\frac{\partial \ell_i[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_{t+1}$$



a)
Loss, $L[\phi]$
b)
Loss, $L[\phi]$
22.5
2.5
ϕ_1
-10
0
10
ϕ_0
No momentum
Momentum

Nesterov accelerated momentum

- Momentum is kind of like a prediction of where we are going

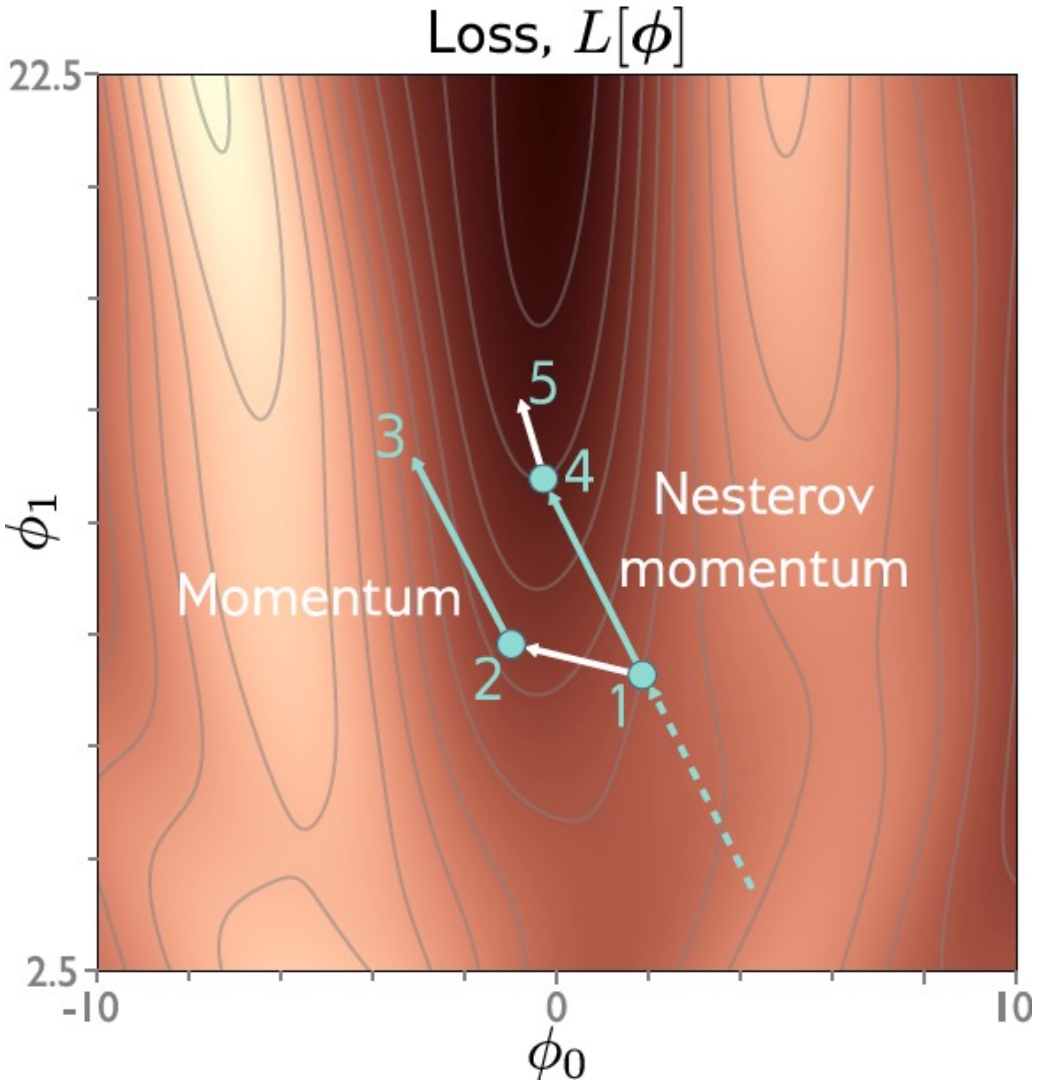
$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta) \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_{t+1}$$

- Move in the predicted direction, THEN, measure the gradient

$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta) \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_t]}{\partial \boldsymbol{\phi}}$$

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_{t+1}$$



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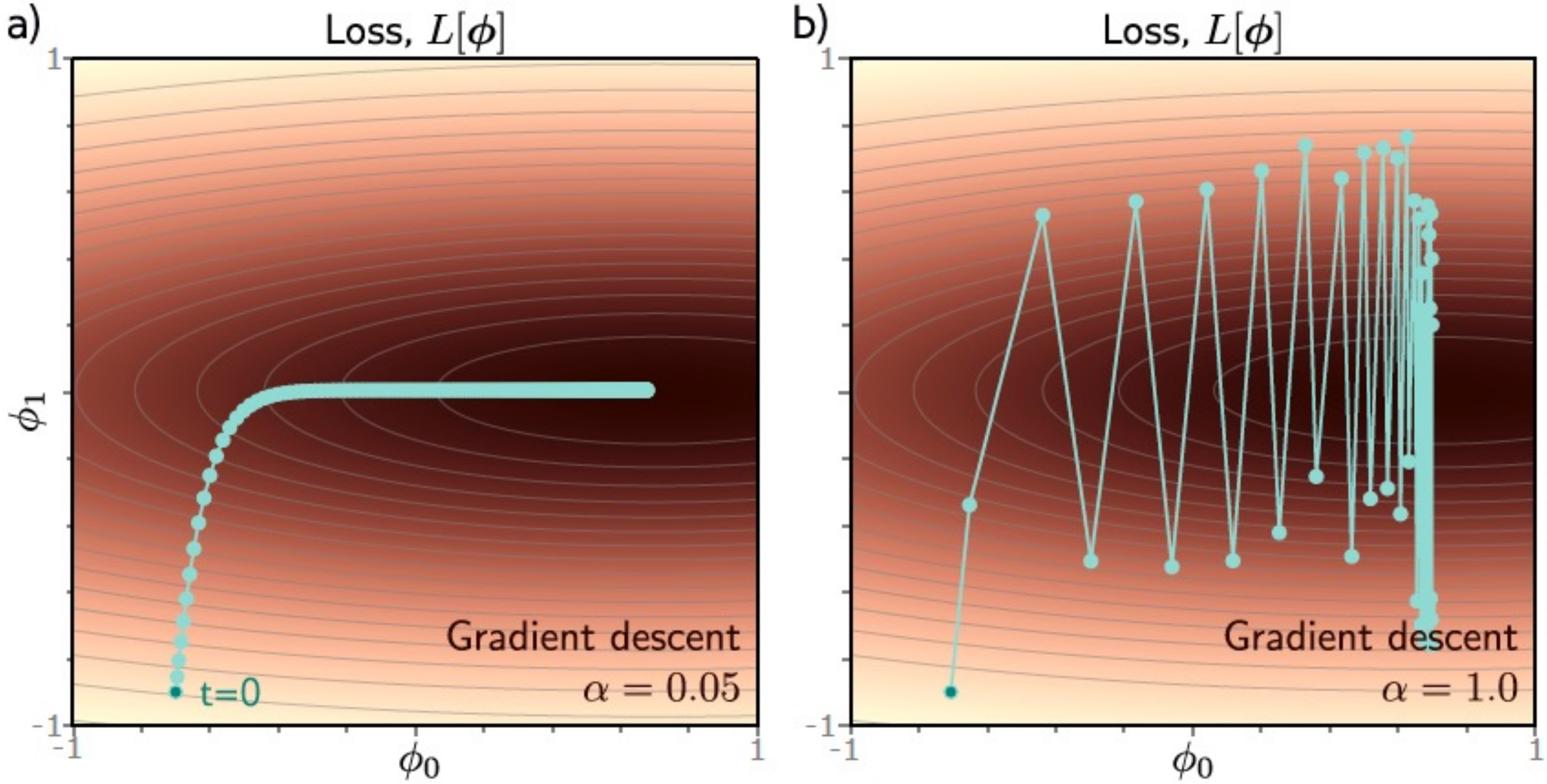
Adaptive moment estimation (Adam)



Normalized gradients

- Measure mean and pointwise squared gradient

$$\mathbf{m}_{t+1} \leftarrow \frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

$$\mathbf{v}_{t+1} \leftarrow \frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}^2$$

- Normalize:

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$

Normalized gradients

- Measure mean and pointwise squared gradient

$$\mathbf{m}_{t+1} \leftarrow \frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

$$\mathbf{v}_{t+1} \leftarrow \frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}^2$$

$$\mathbf{m}_{t+1} = \begin{bmatrix} 3.0 \\ -2.0 \\ 5.0 \end{bmatrix}$$

$$\mathbf{v}_{t+1} = \begin{bmatrix} 9.0 \\ 4.0 \\ 25.0 \end{bmatrix}$$

- Normalize:

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$

$$\frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon} = \begin{bmatrix} 1.0 \\ -1.0 \\ 1.0 \end{bmatrix}$$

Normalized gradients

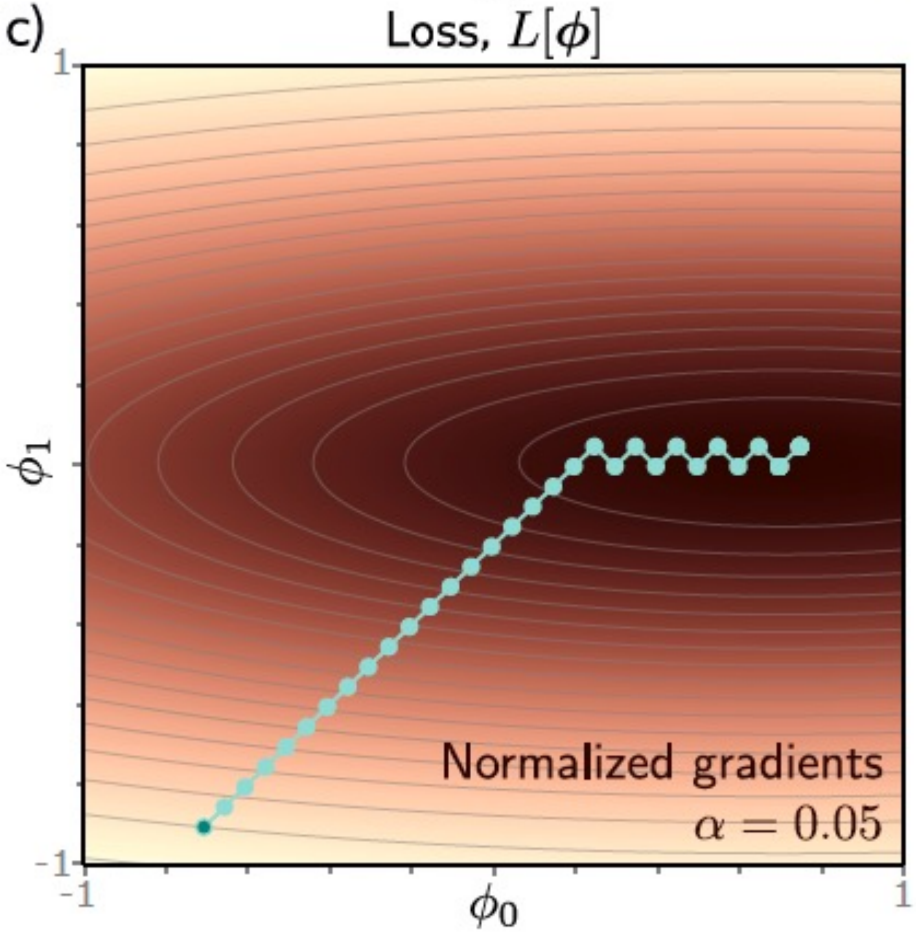
- Measure mean and pointwise squared gradient

$$\mathbf{m}_{t+1} \leftarrow \frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

$$\mathbf{v}_{t+1} \leftarrow \frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}^2$$

- Normalize:

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$



Adaptive moment estimation (Adam)

- Compute mean and pointwise squared gradients with momentum

$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta)\frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

$$\mathbf{v}_{t+1} \leftarrow \gamma \cdot \mathbf{v}_t + (1-\gamma)\left(\frac{\partial L[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}\right)^2$$

- Moderate near start of the sequence

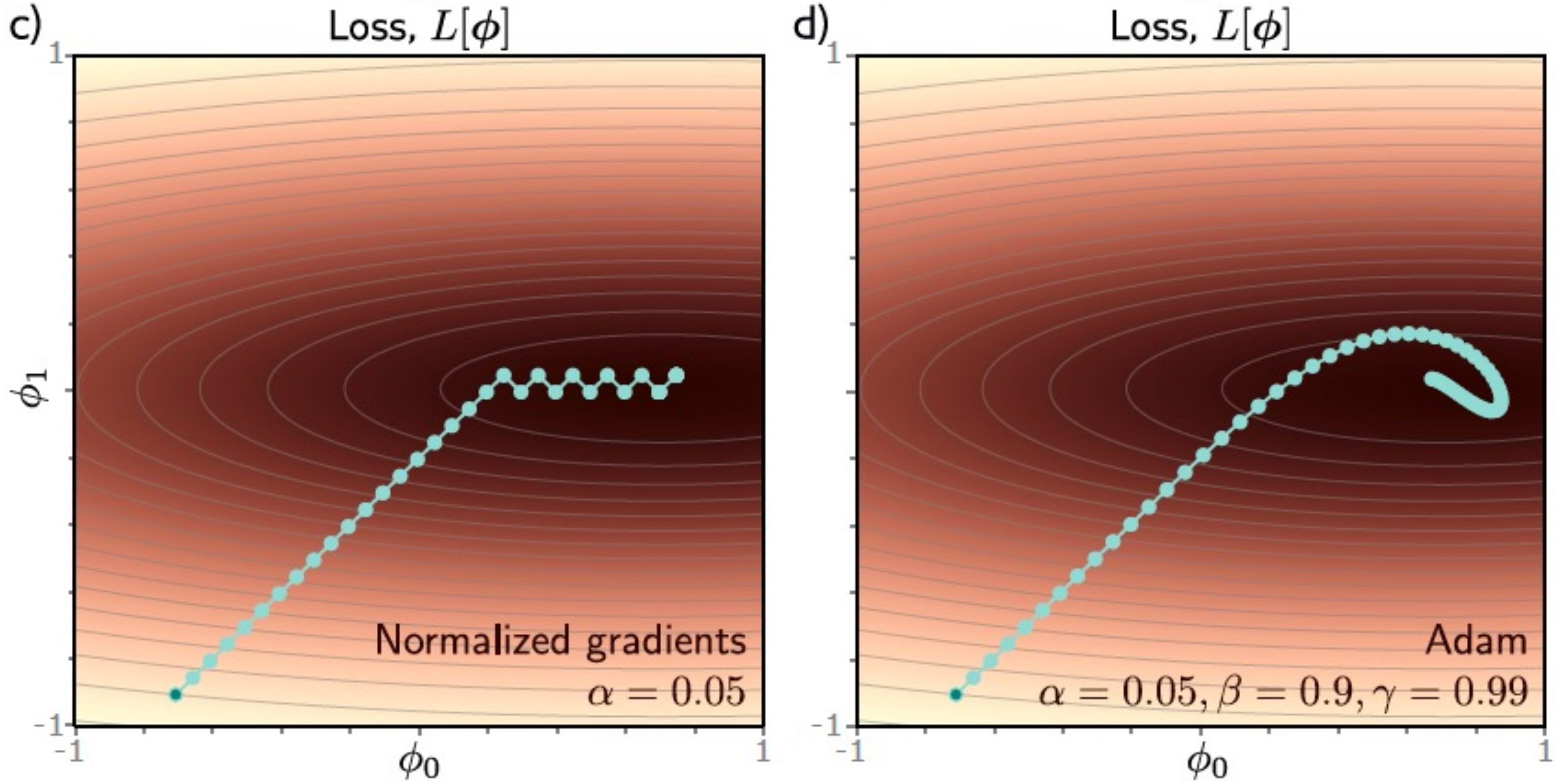
$$\tilde{\mathbf{m}}_{t+1} \leftarrow \frac{\mathbf{m}_{t+1}}{1-\beta^{t+1}}$$

$$\tilde{\mathbf{v}}_{t+1} \leftarrow \frac{\mathbf{v}_{t+1}}{1-\gamma^{t+1}}$$

- Update the parameters

$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \frac{\tilde{\mathbf{m}}_{t+1}}{\sqrt{\tilde{\mathbf{v}}_{t+1}} + \epsilon}$$

Adaptive moment estimation (Adam)



Hyperparameters

- Choice of learning algorithm
- Learning rate
- Momentum