Deep Learning for Data Science
DS 542

https://dl4ds.github.io/fa2025/

Fitting Models

Original slides by Tom Gardos,
other content from Understanding Deep Learning unless otherwise cited

Plan for Today

- Homework 3 post-mortem
- Gradient descent review
- Stochastic gradient descent (more formally)
- Momentum
- Adam

Homework 3 Post-Mortem

Raise your hand if you encountered any of the following.

- Bad prediction accuracy
- Loss function improving very slowly
- Loss function going up
- NaN or infinity in loss calculations
- NaN in initial loss calculations?

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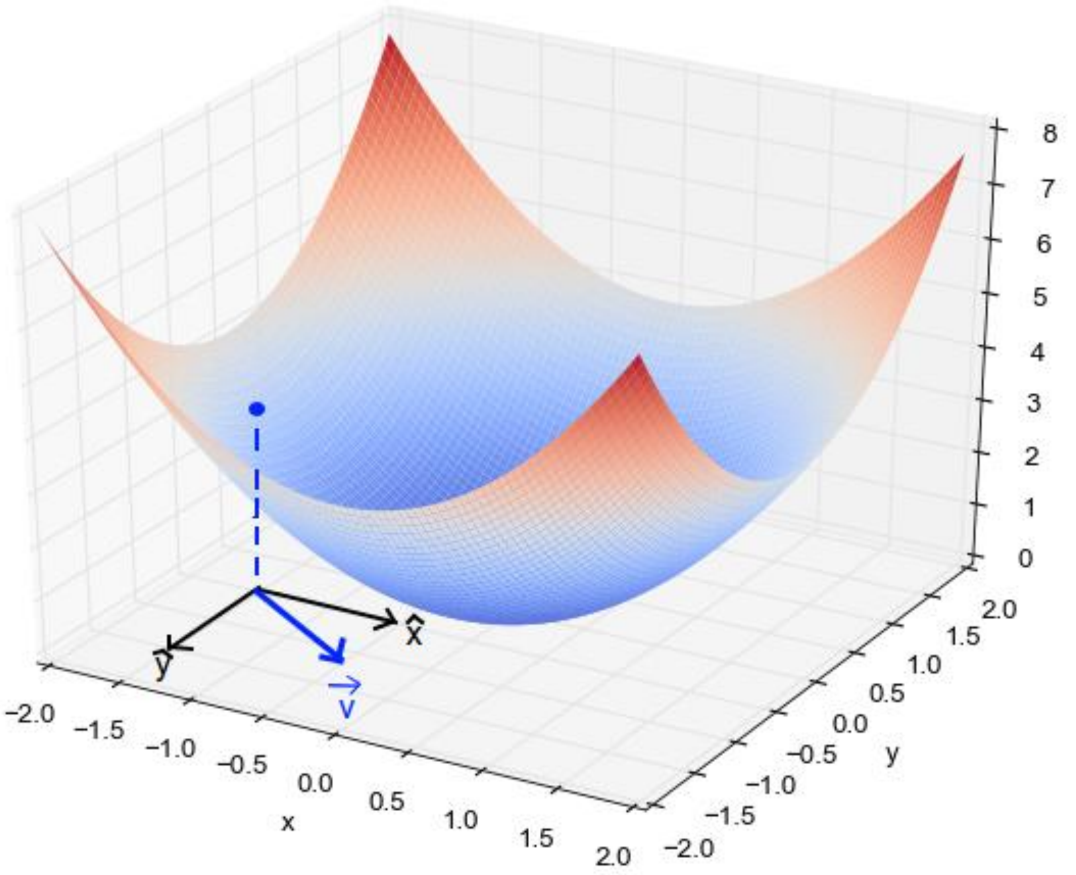
Gradient

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

Partial derivative, e.g. rate of change, w.r.t. each input (independent) variable.



Geometric Interpretation: Each variable is a unit vector, and then

- gradient is the rate of change (increase) in the direction of each unit vector
- vector sum points to the overall direction of greatest change (increase)

Gradient descent algorithm

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

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

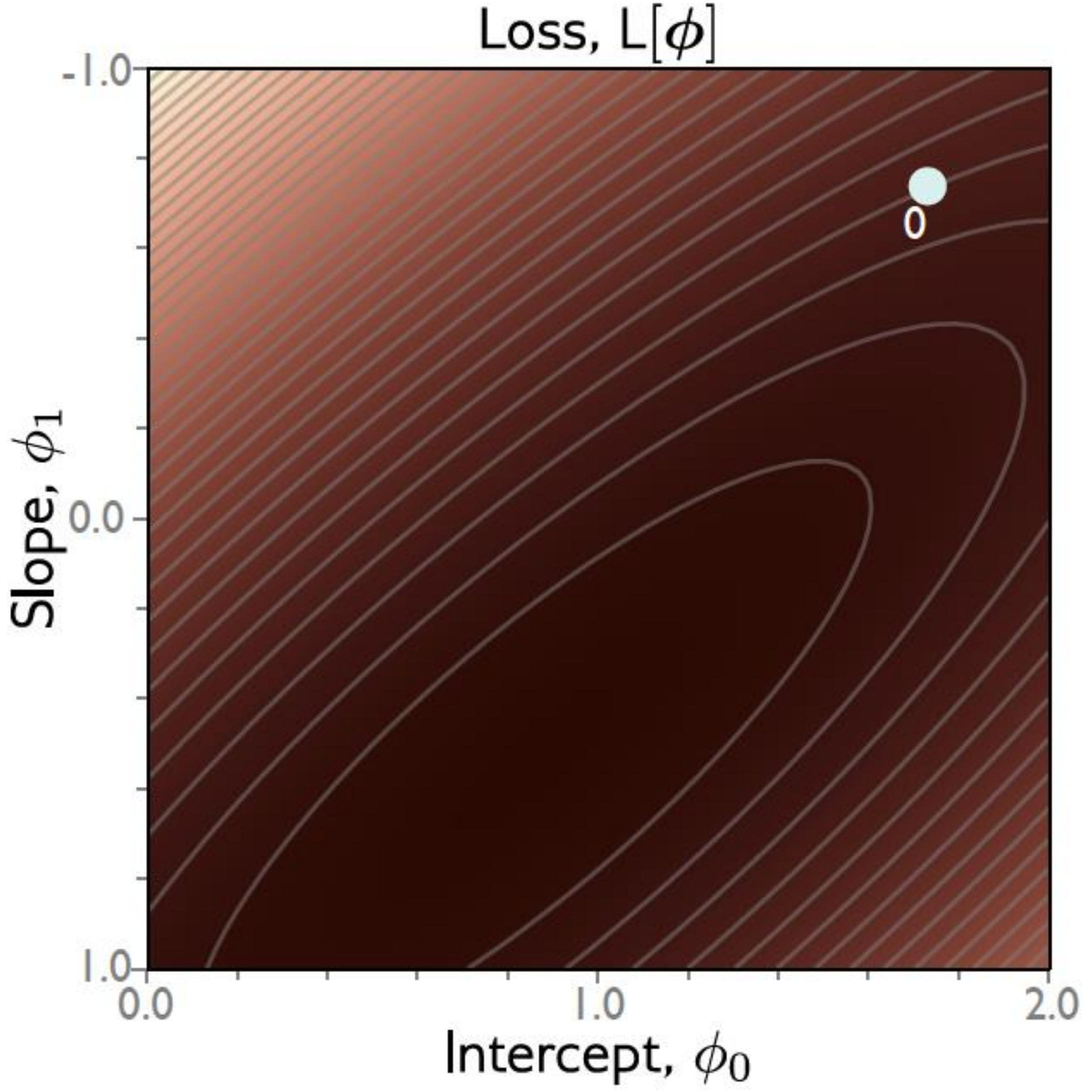
Also notated as $\nabla_w L$

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.

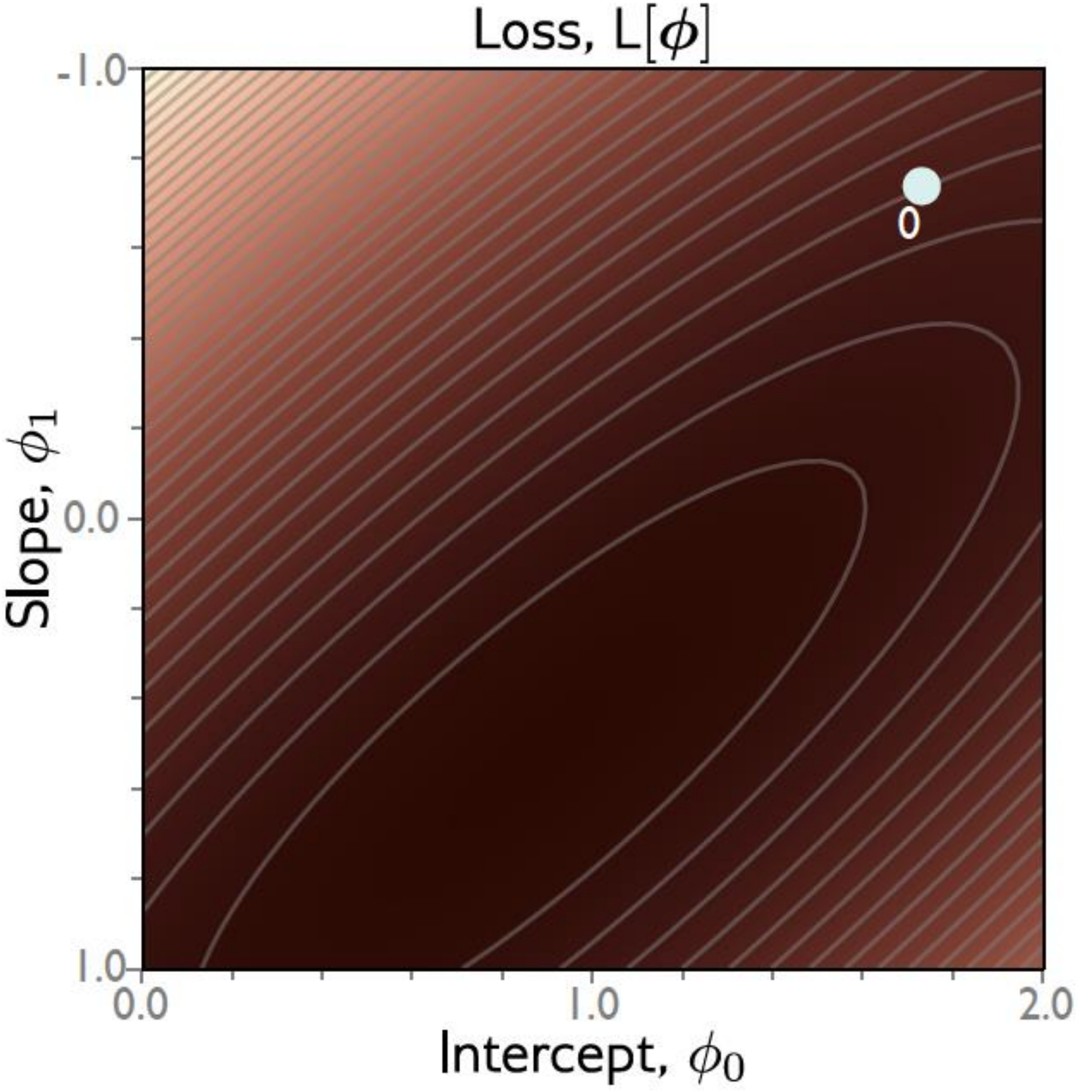
Gradient descent



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

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

Gradient descent



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\end{aligned}
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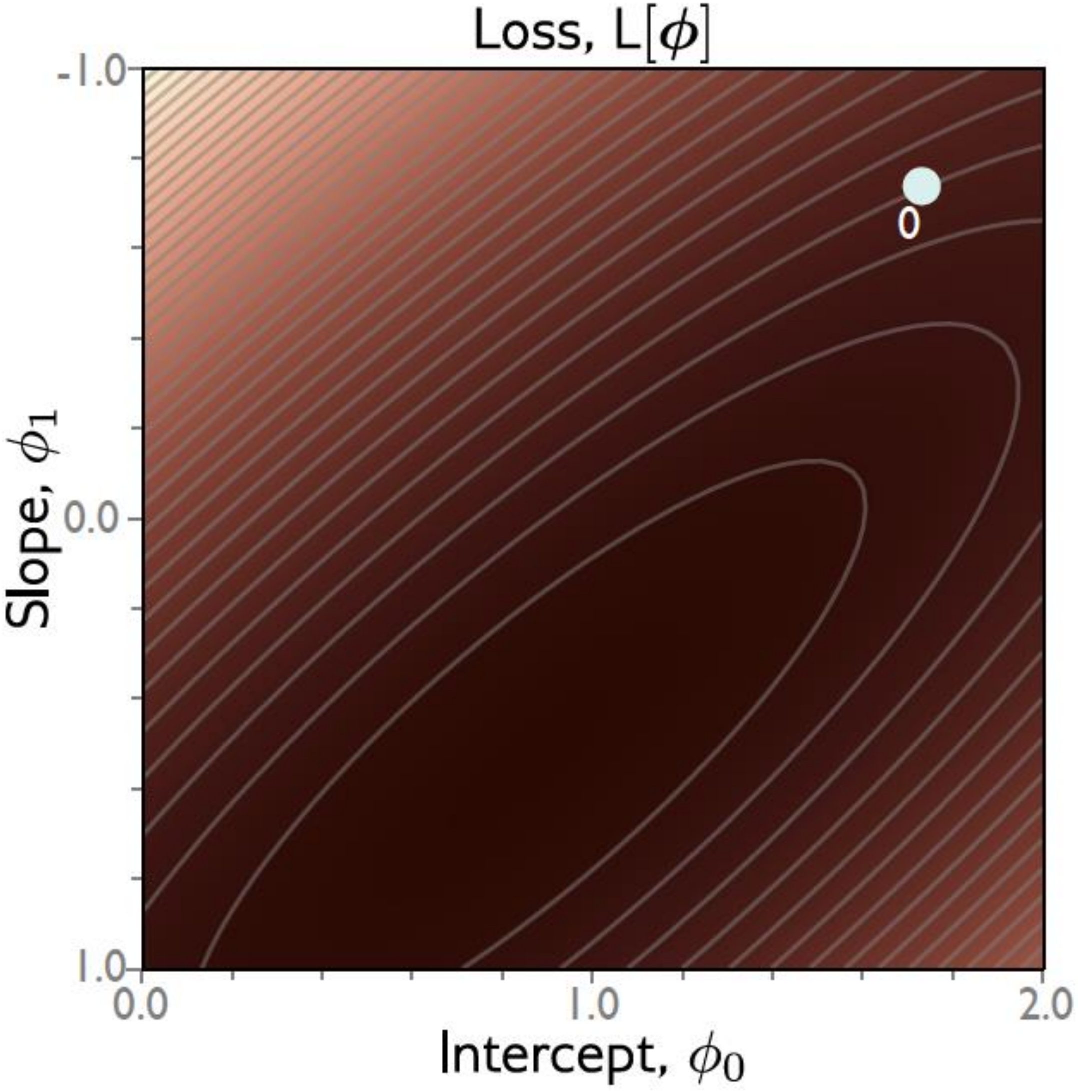
$$
\frac{\partial L}{\partial \boldsymbol{\phi}} = \frac{\partial}{\partial \boldsymbol{\phi}} \sum_{i=1}^{I} \ell_i = \sum_{i=1}^{I} \frac{\partial \ell_i}{\partial \boldsymbol{\phi}}
$$

Gradient descent



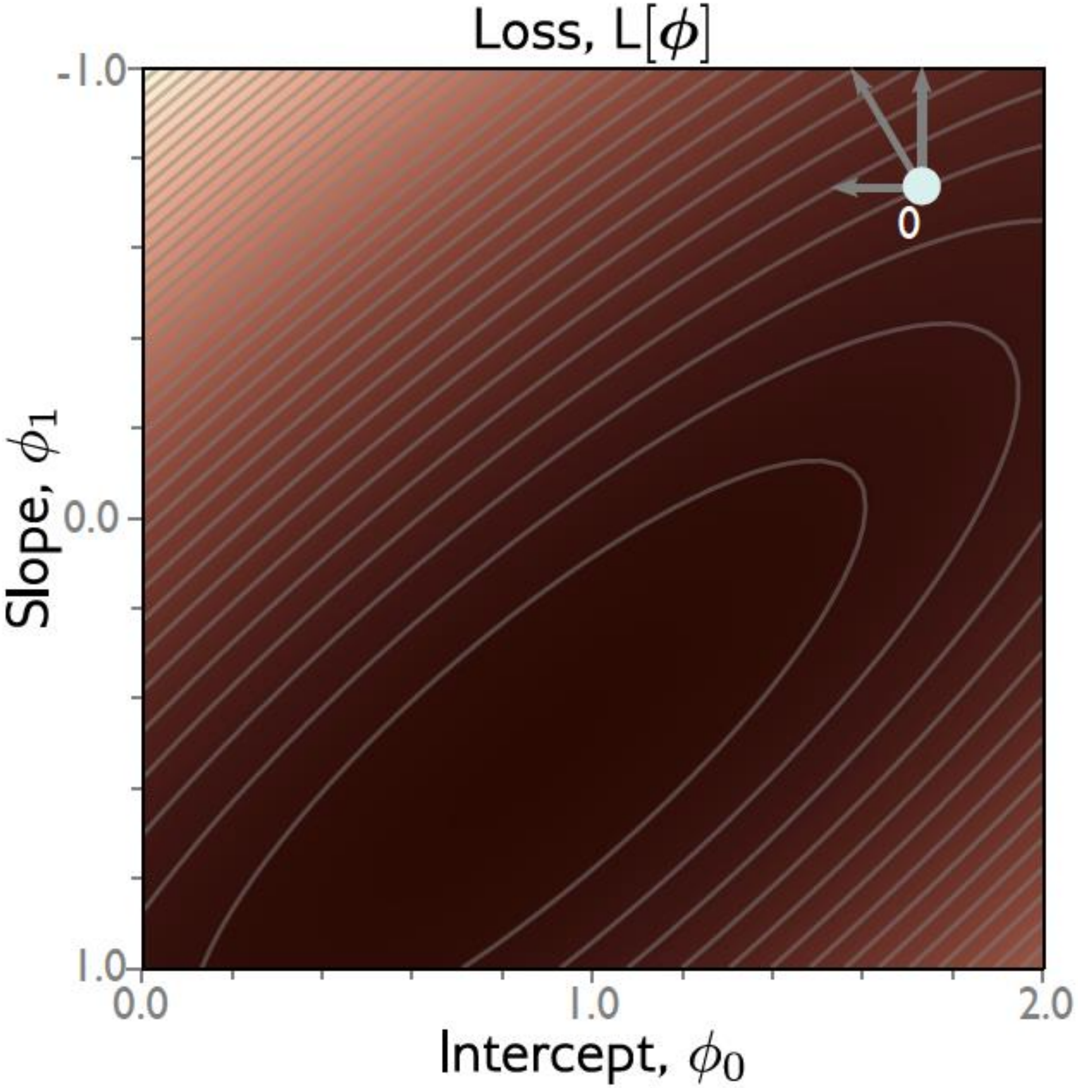
Step 1: Compute derivatives (slopes of function) with Respect to the parameters

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

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

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

Gradient descent



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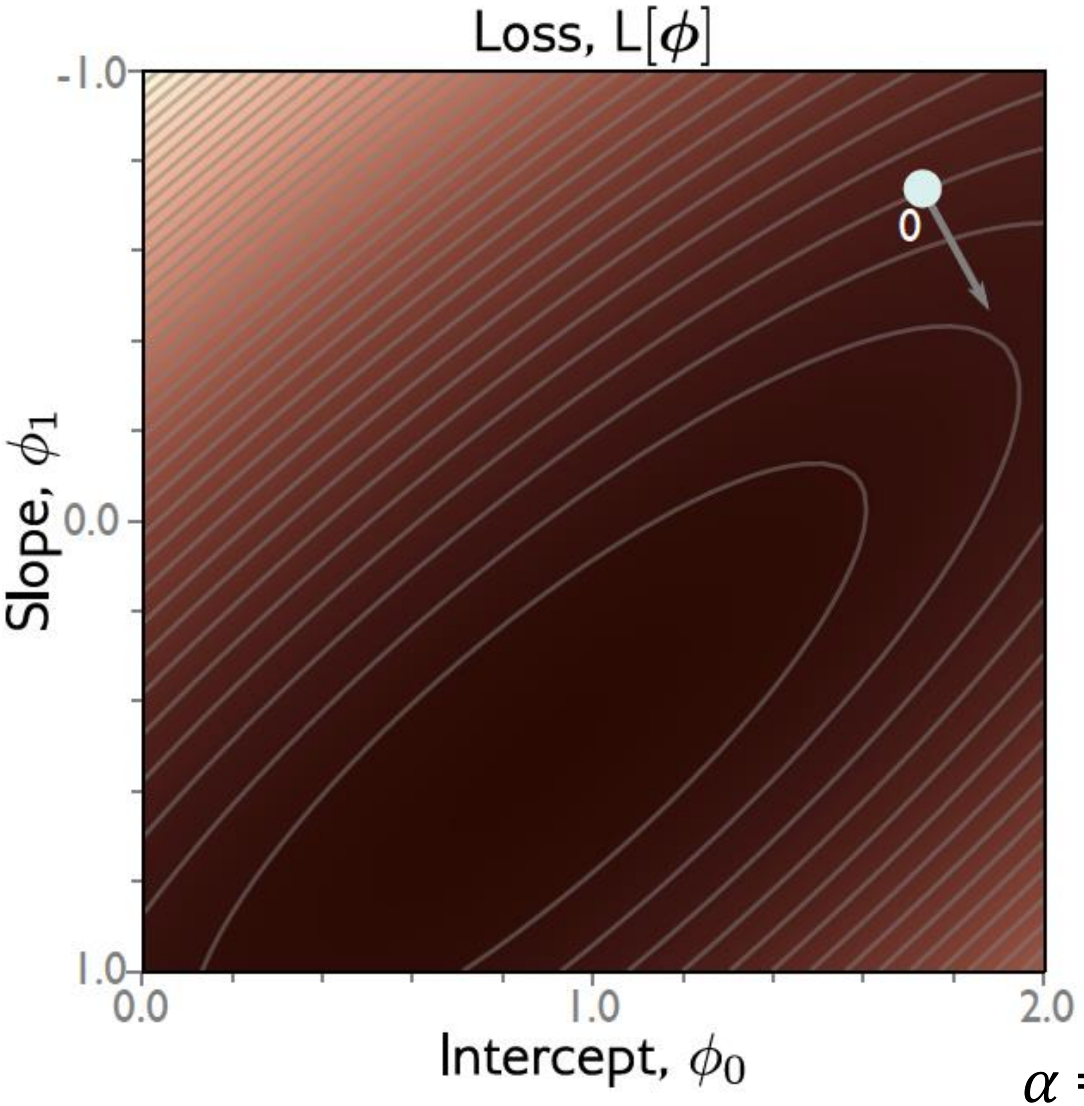

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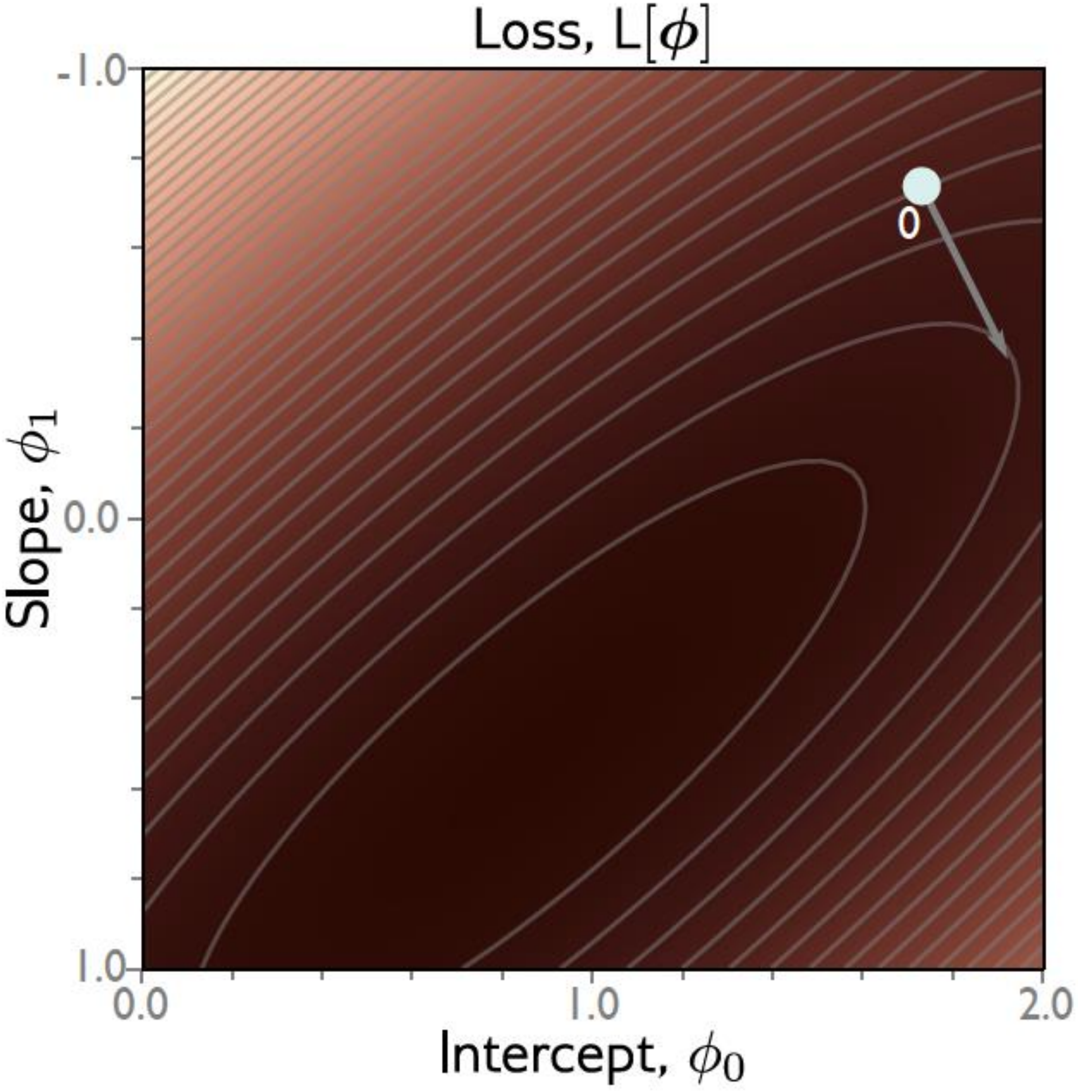
Step 2: Update parameters according to rule

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

α = step size or learning rate if fixed

Gradient descent



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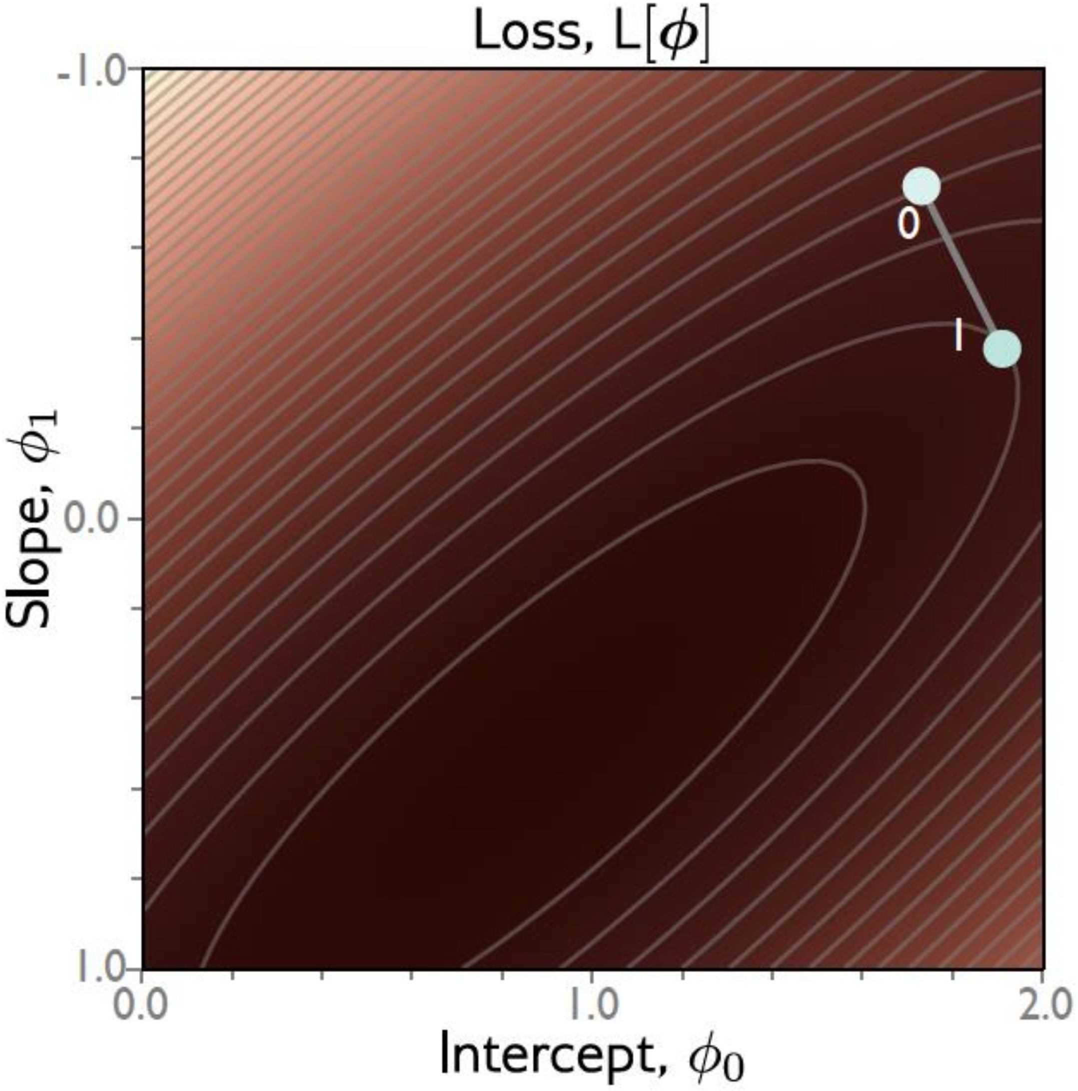
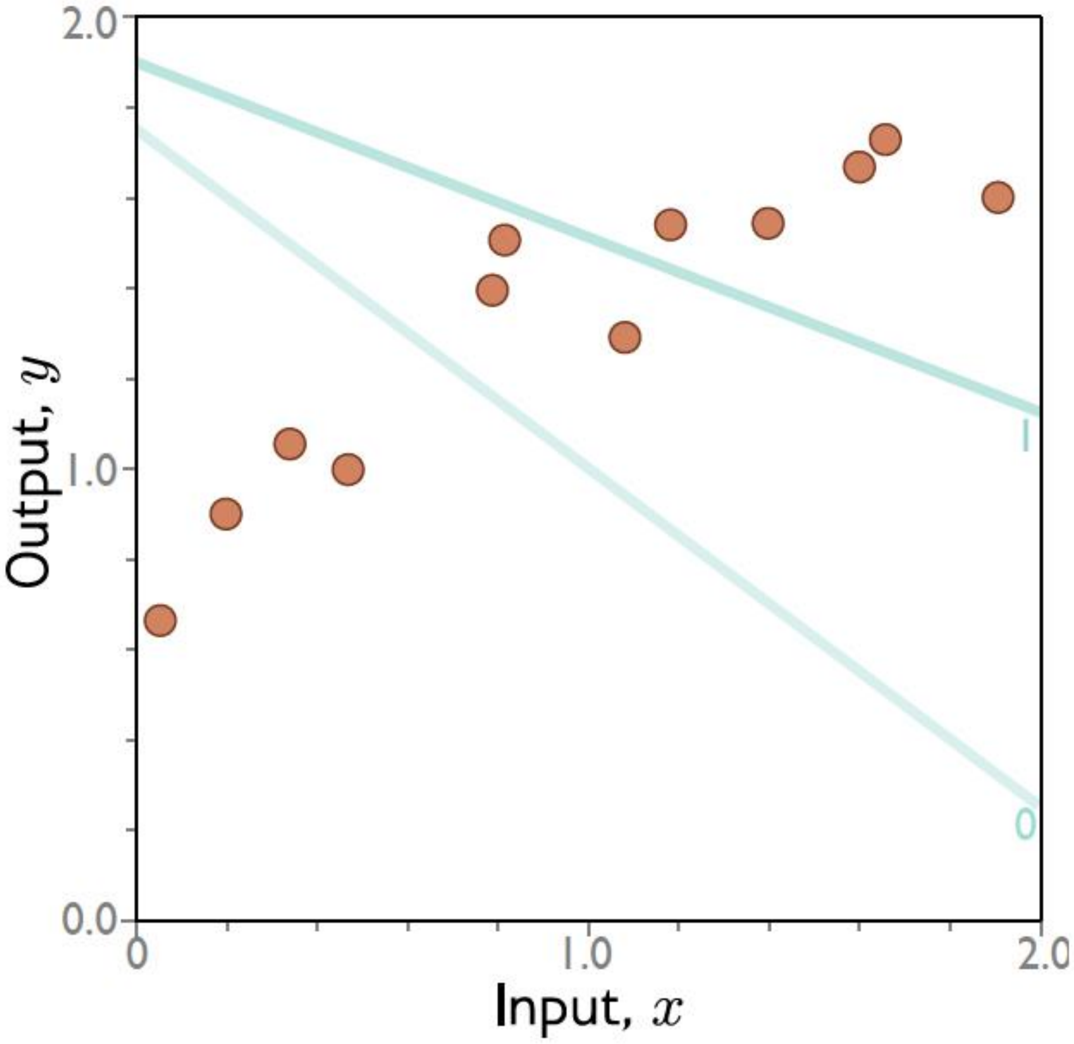
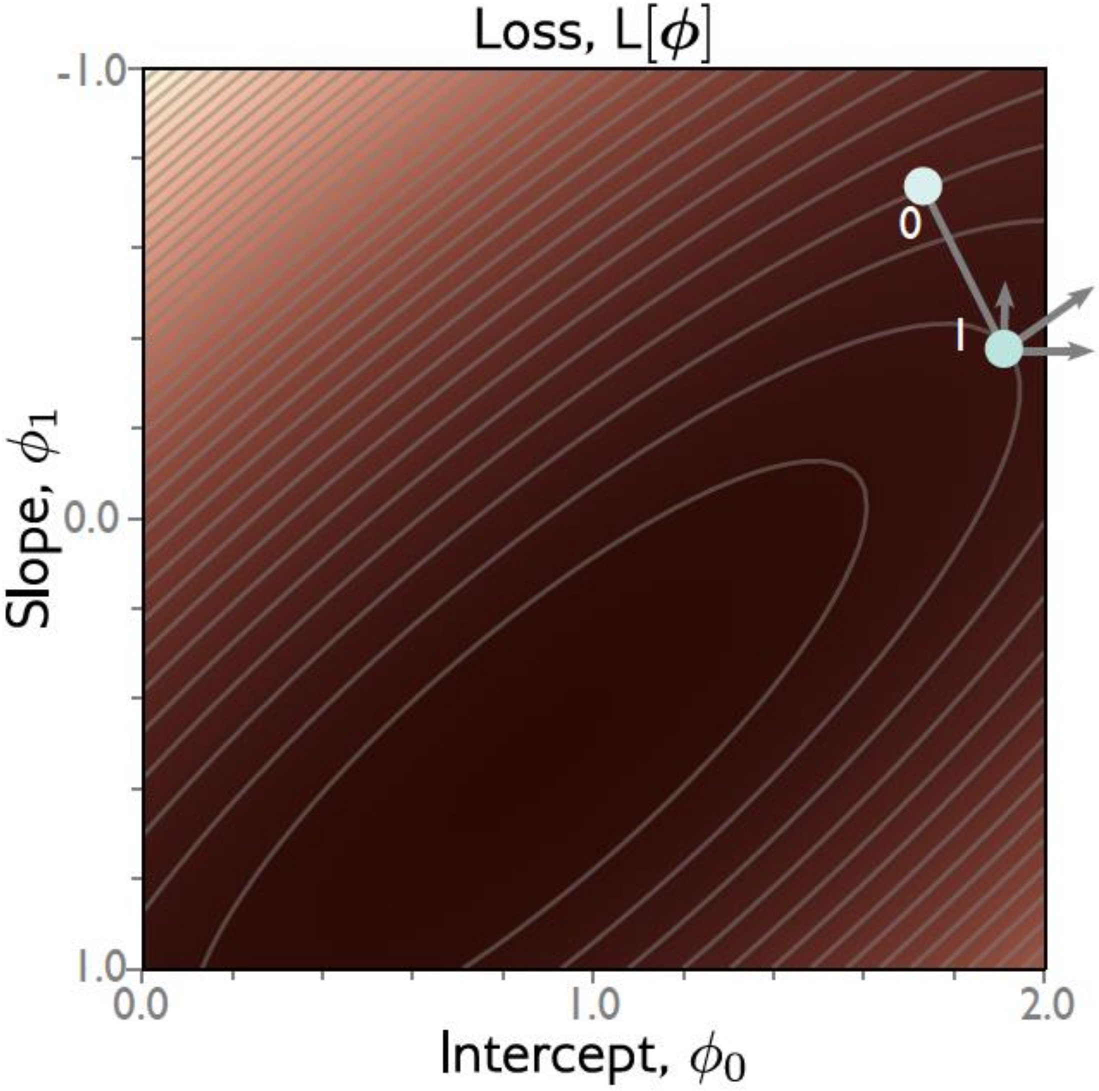
Gradient descent





Gradient descent



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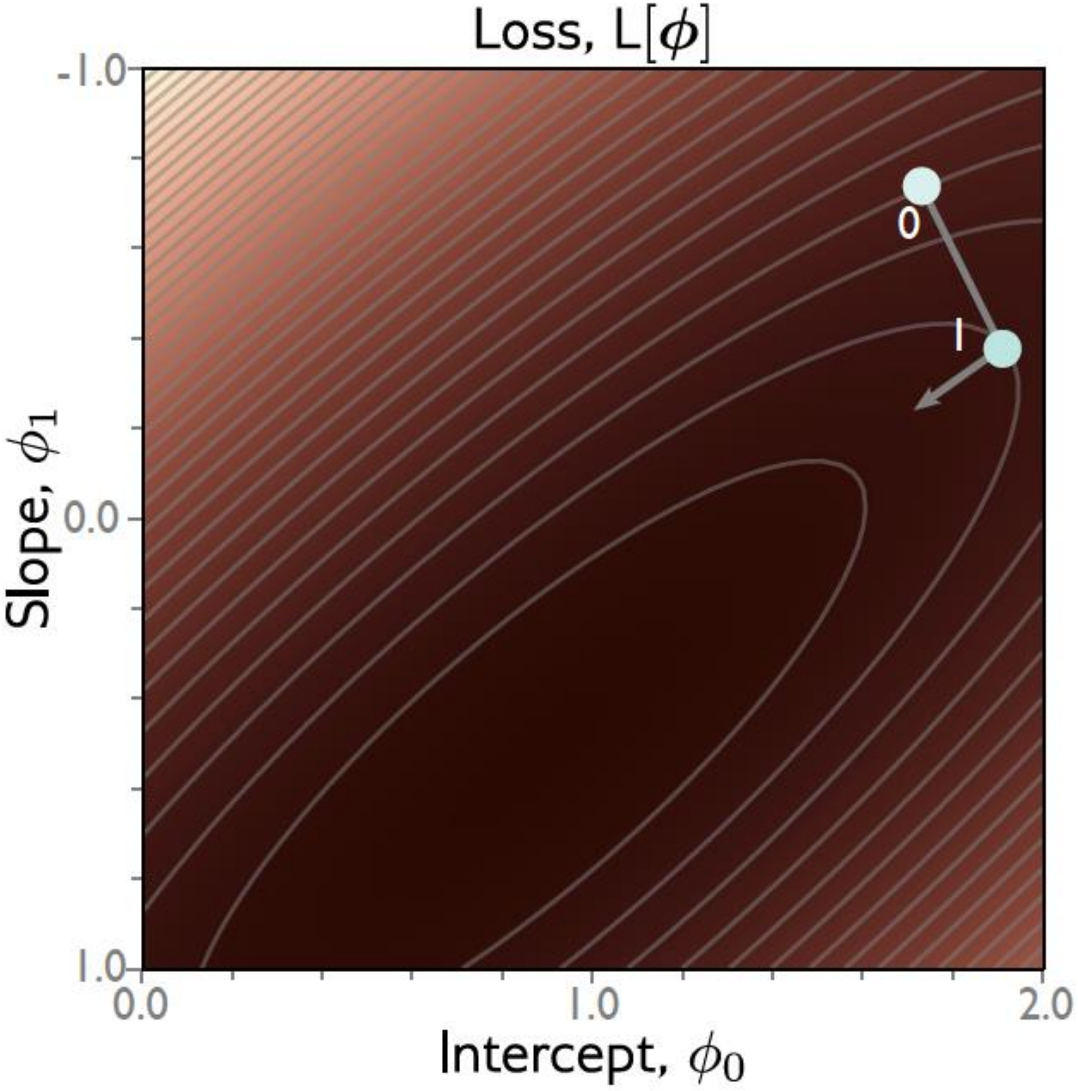

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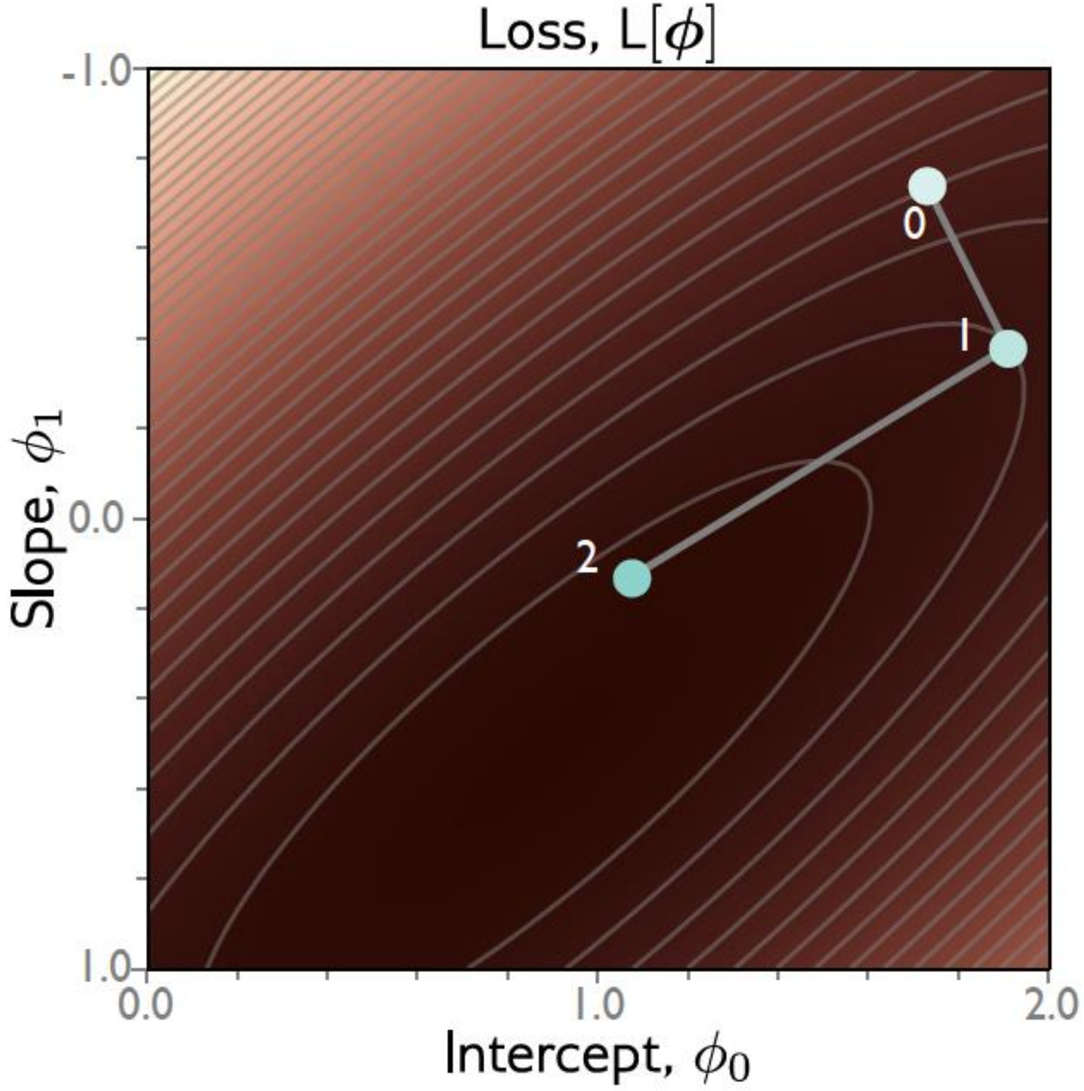
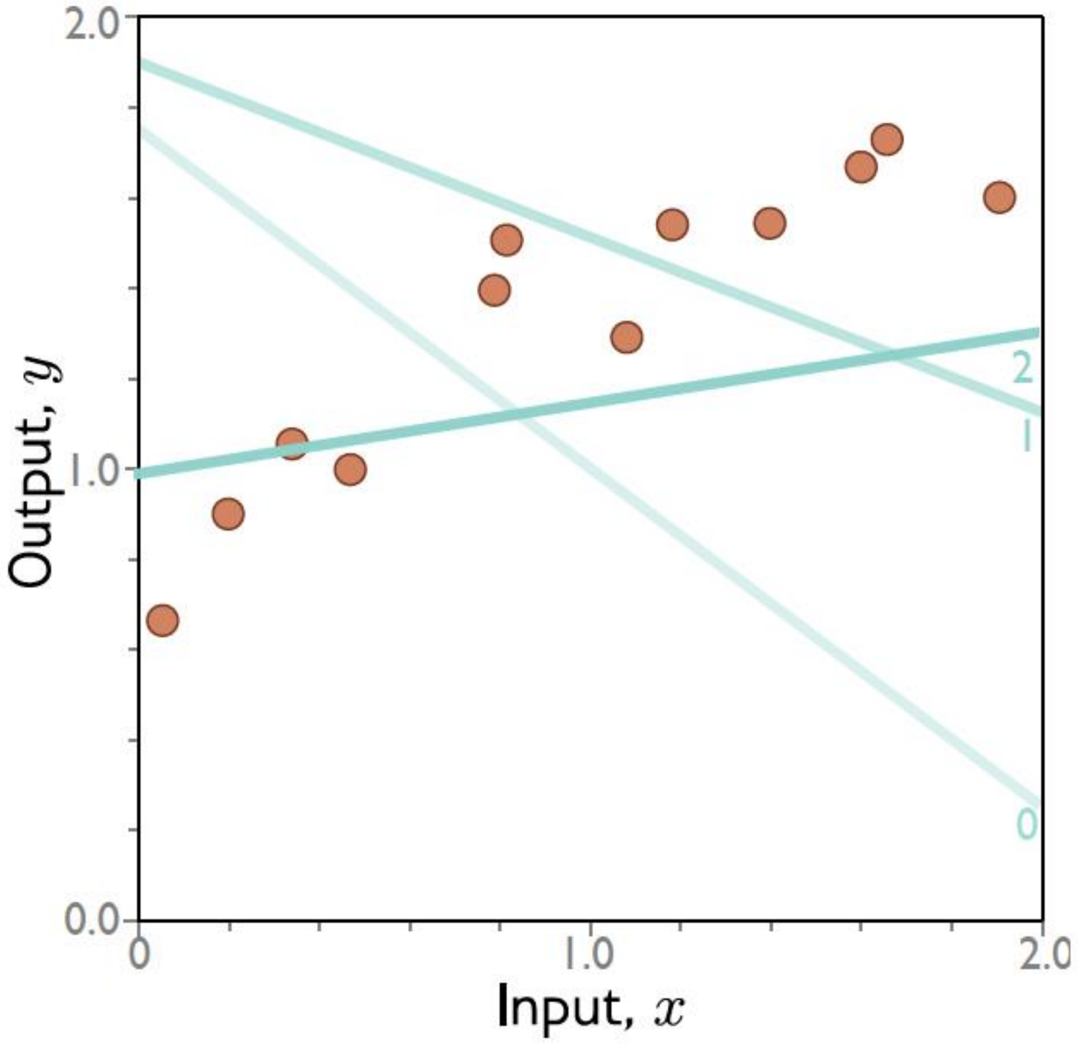
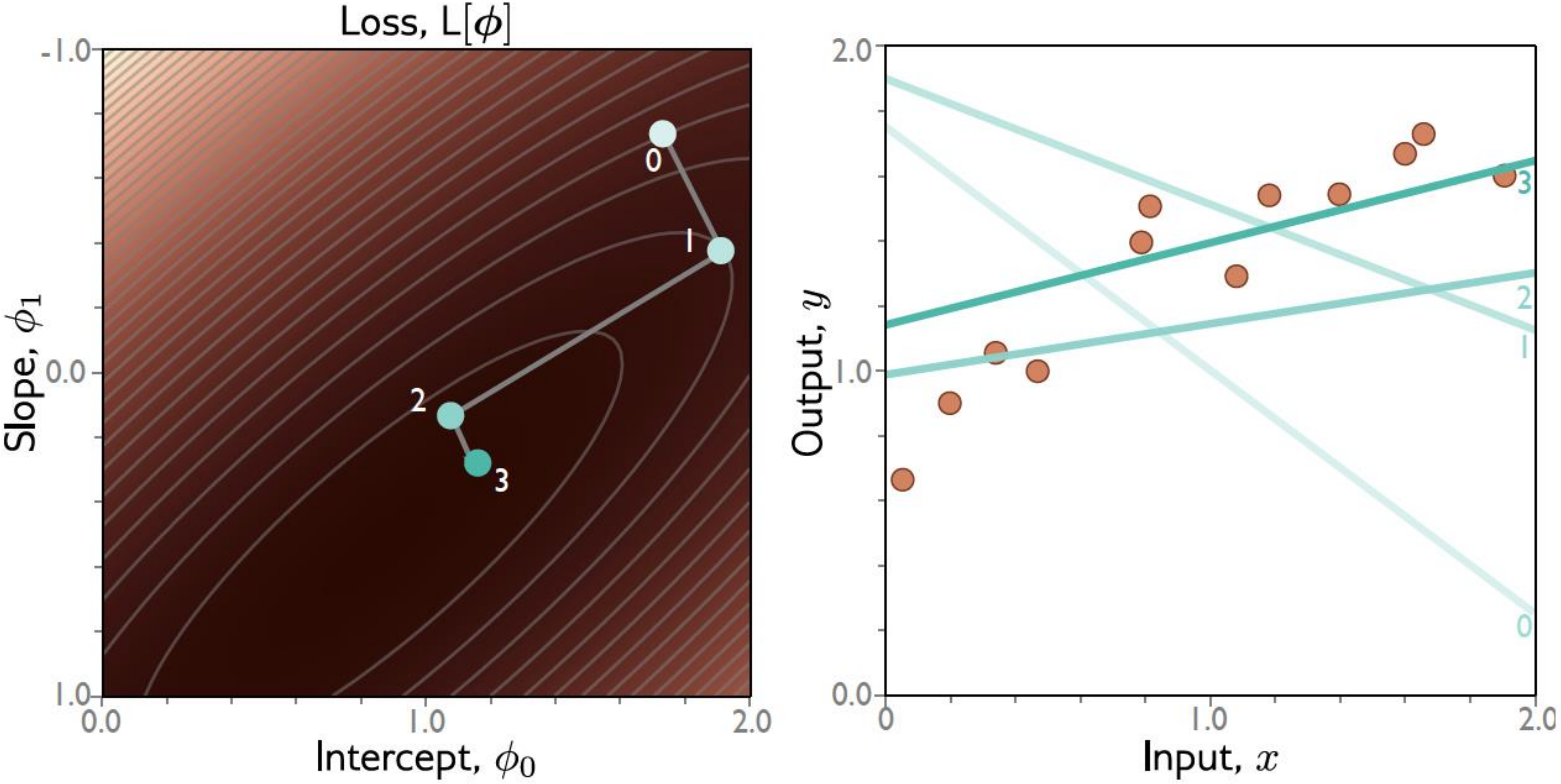
Gradient descent

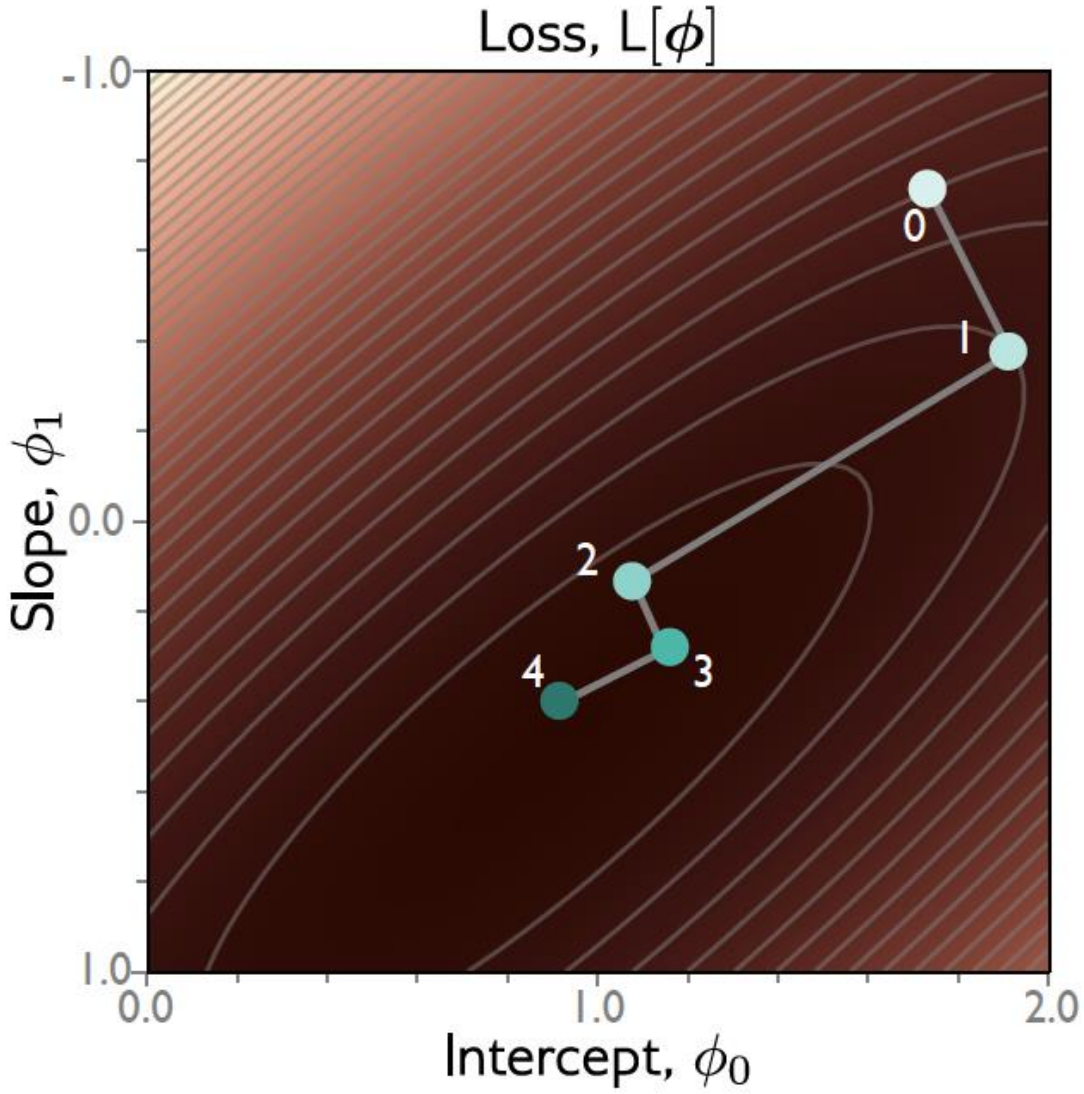


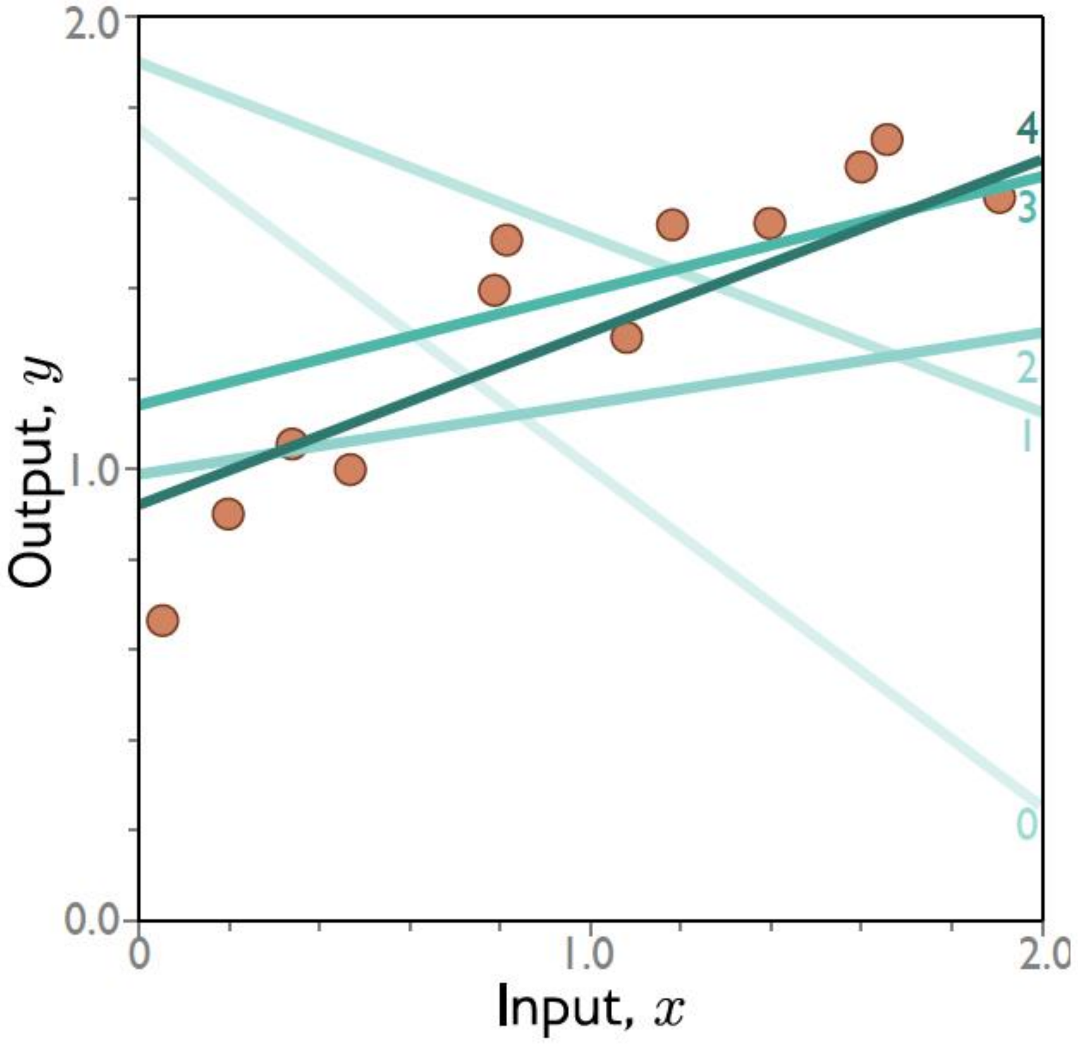


Gradient descent



Gradient descent





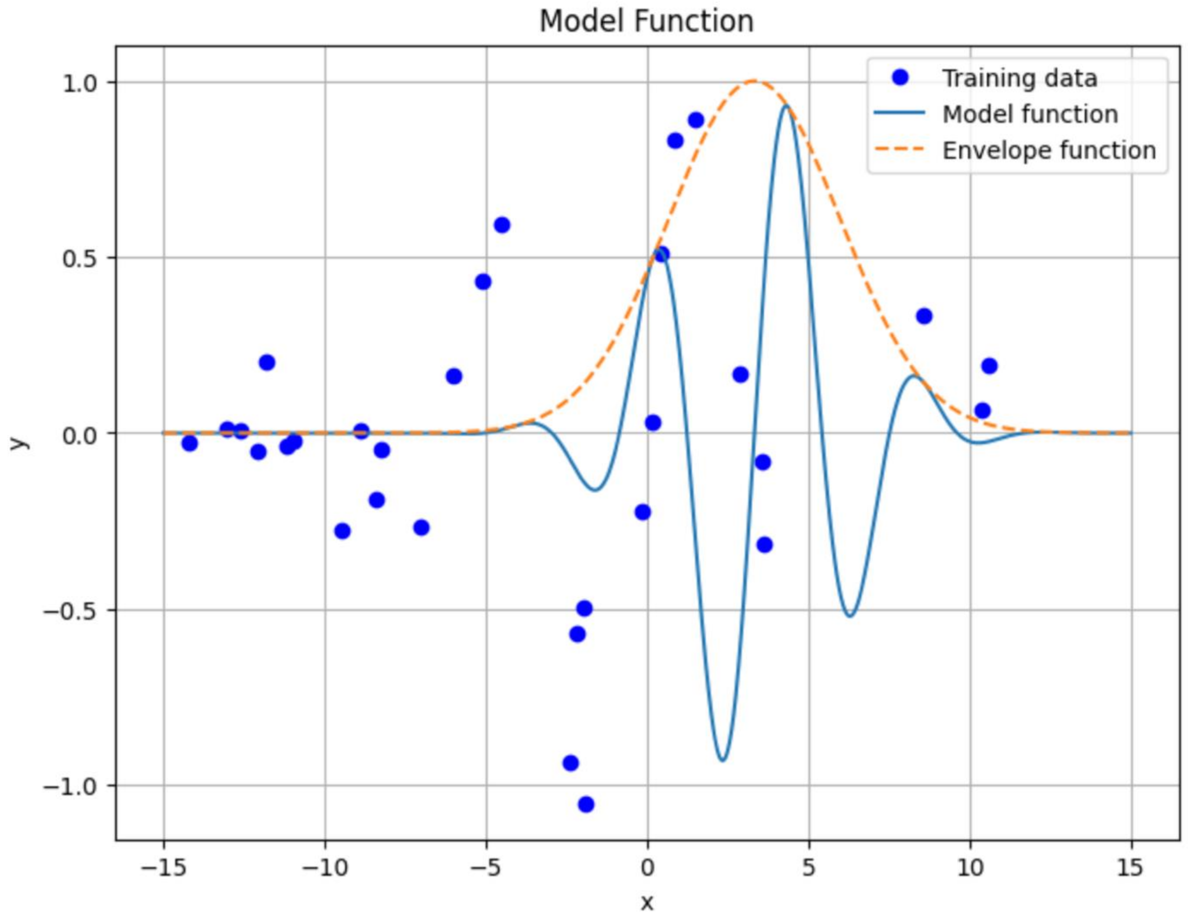
The linear model loss function was convex.

We’ll use a more complex (non-convex) model that we can still visualize in 2D and 3D

➔ Gabor Function

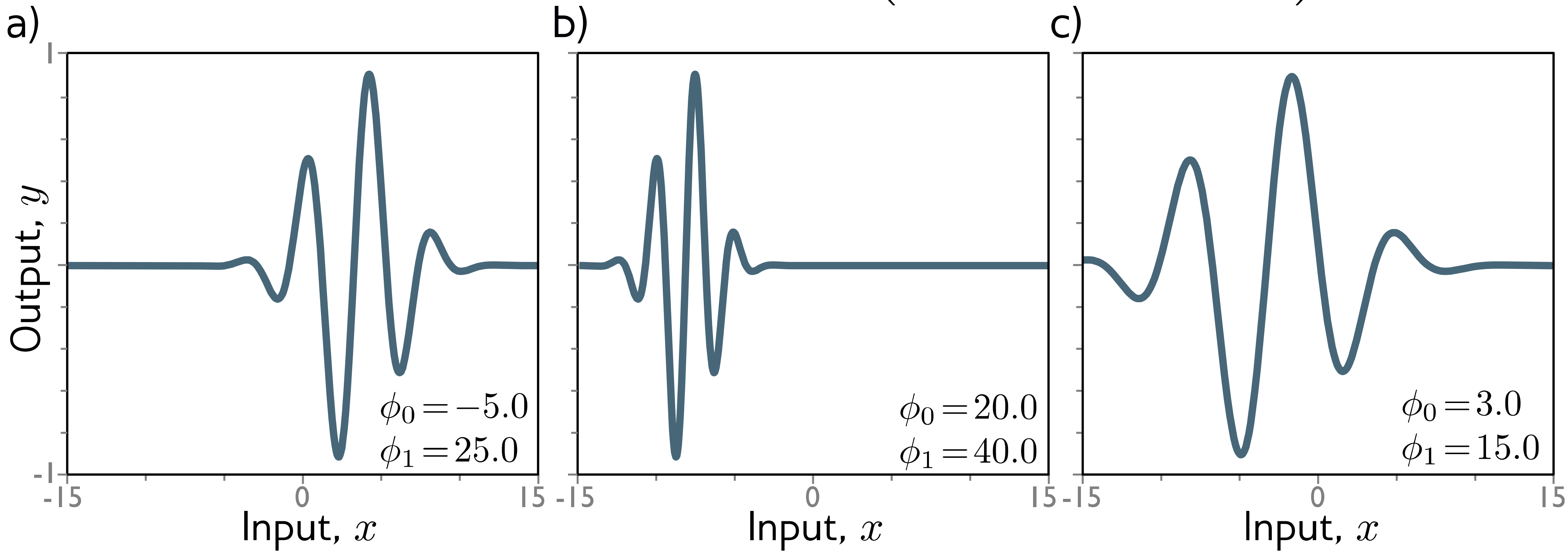
Gabor Model (with Envelope)

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



Gabor model

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

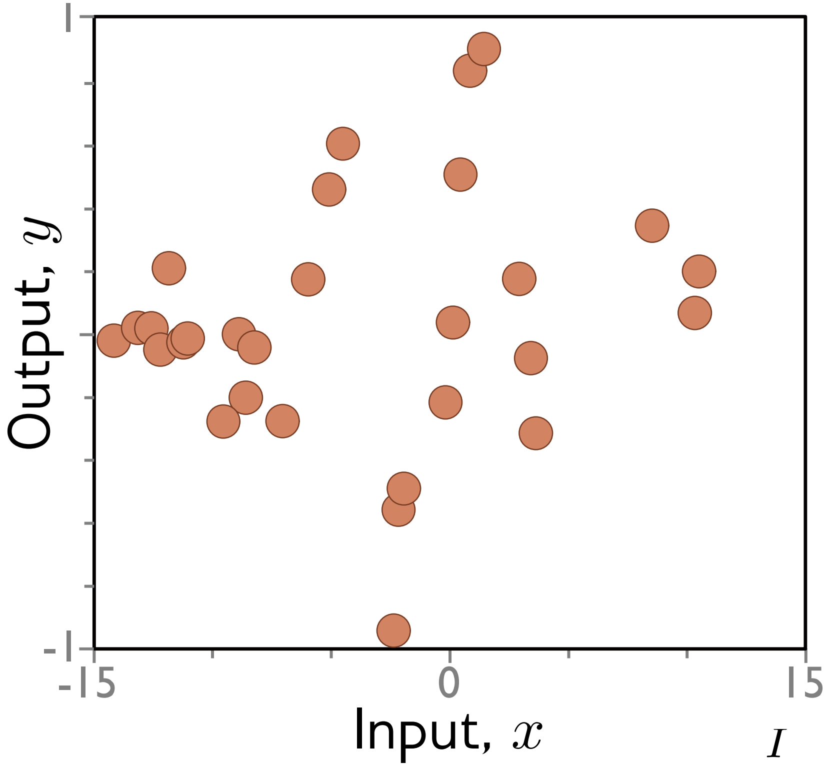


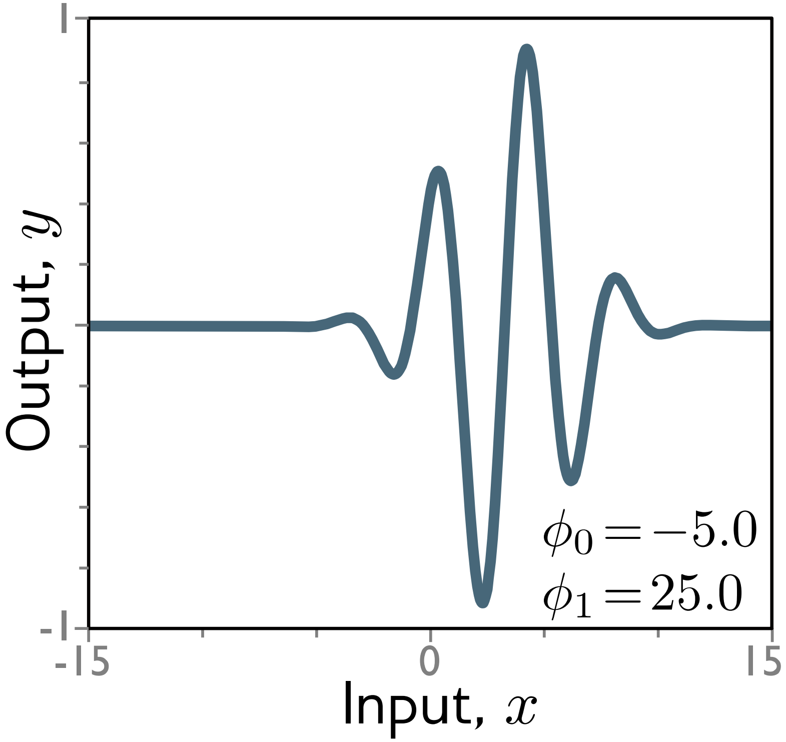
ϕ_0 shifts left and right

ϕ_1 shrinks and expands the sinusoid and envelope

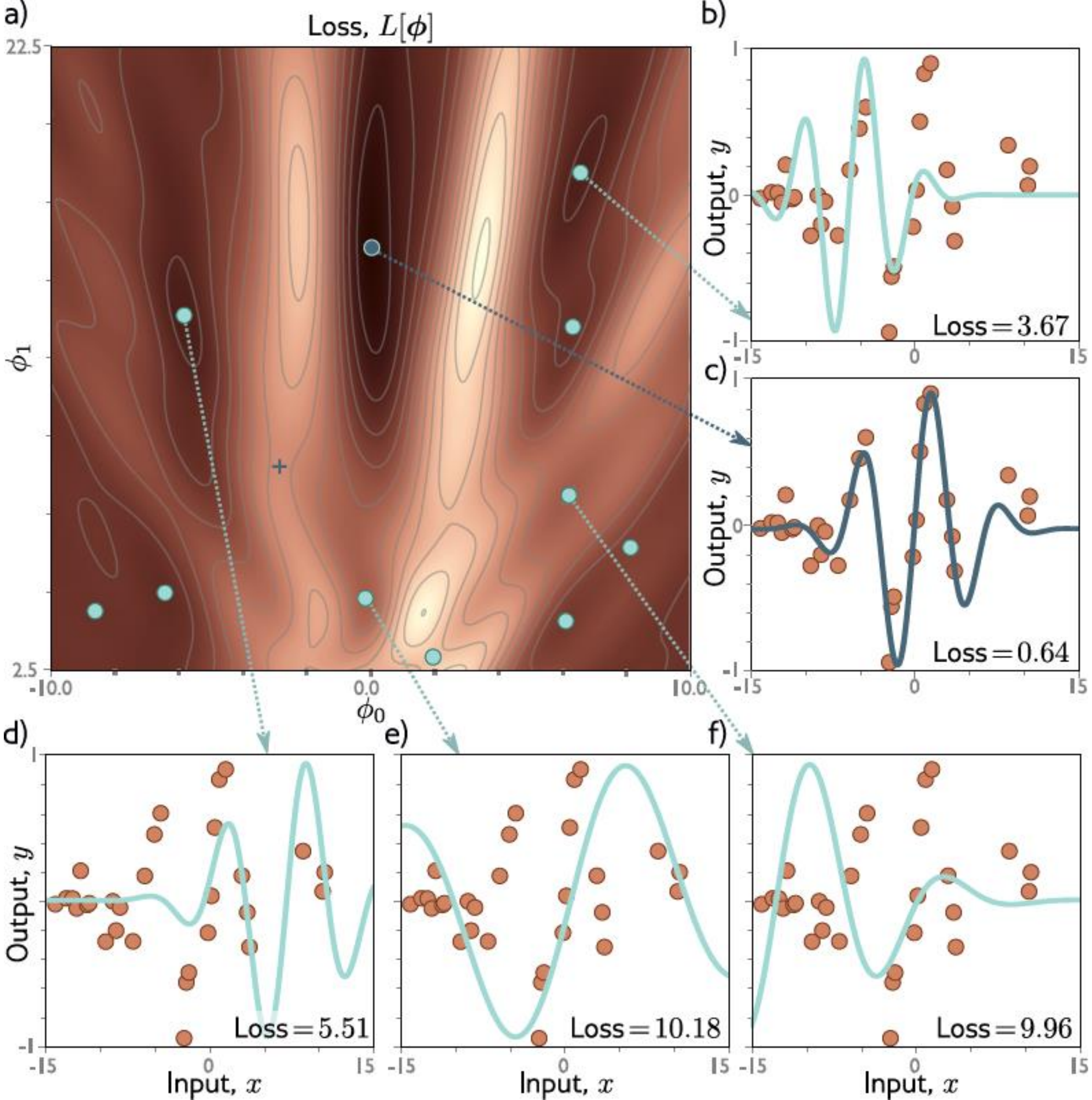
Toy Dataset and Gabor model

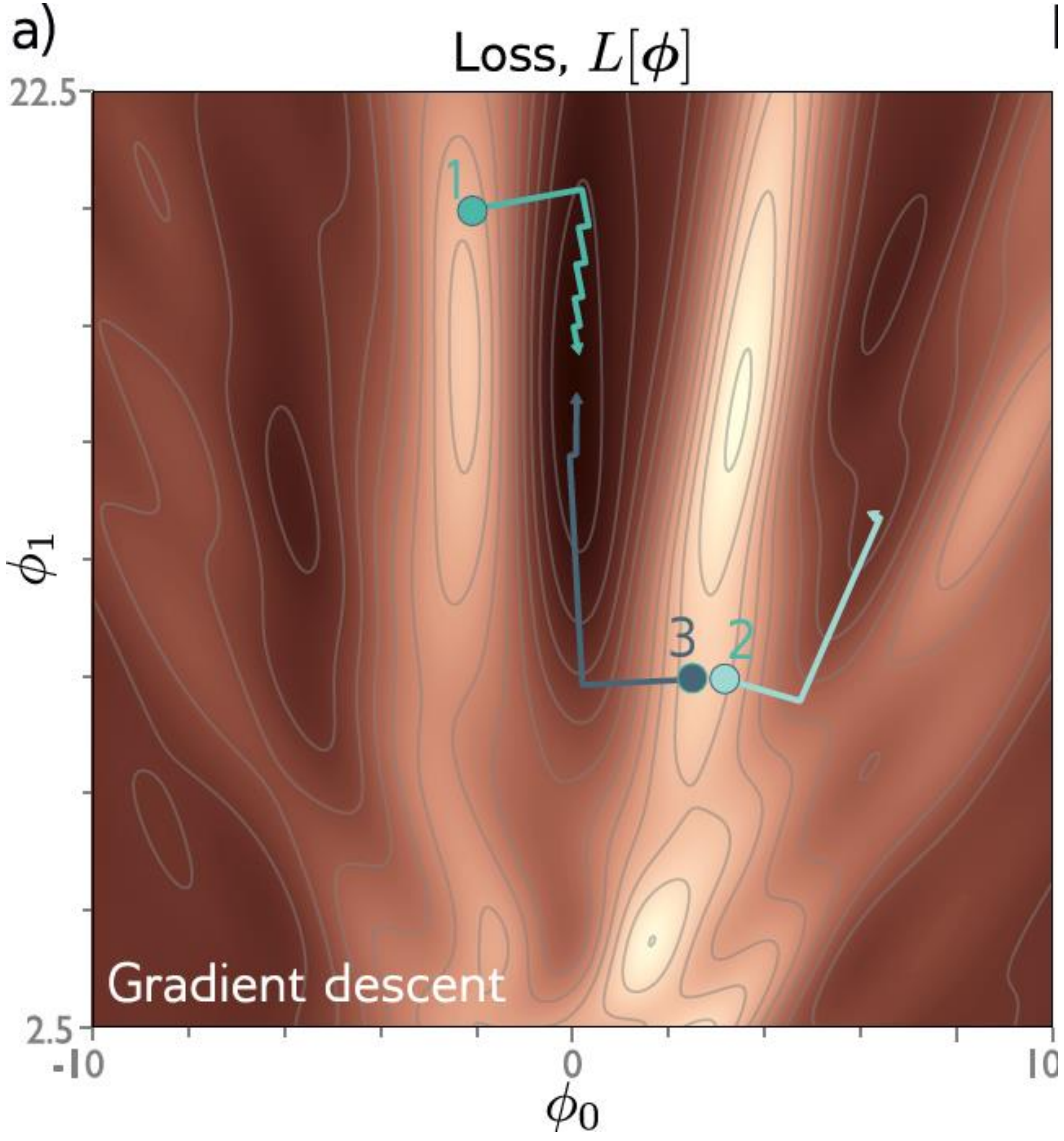
$$\mathrm{f}[x, \boldsymbol{\phi}] = \sin[\phi_0 + 0.06 \cdot \phi_1 x] \cdot \exp\left(-\frac{(\phi_0 + 0.06 \cdot \phi_1 x)^2}{8.0}\right)$$





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


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



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

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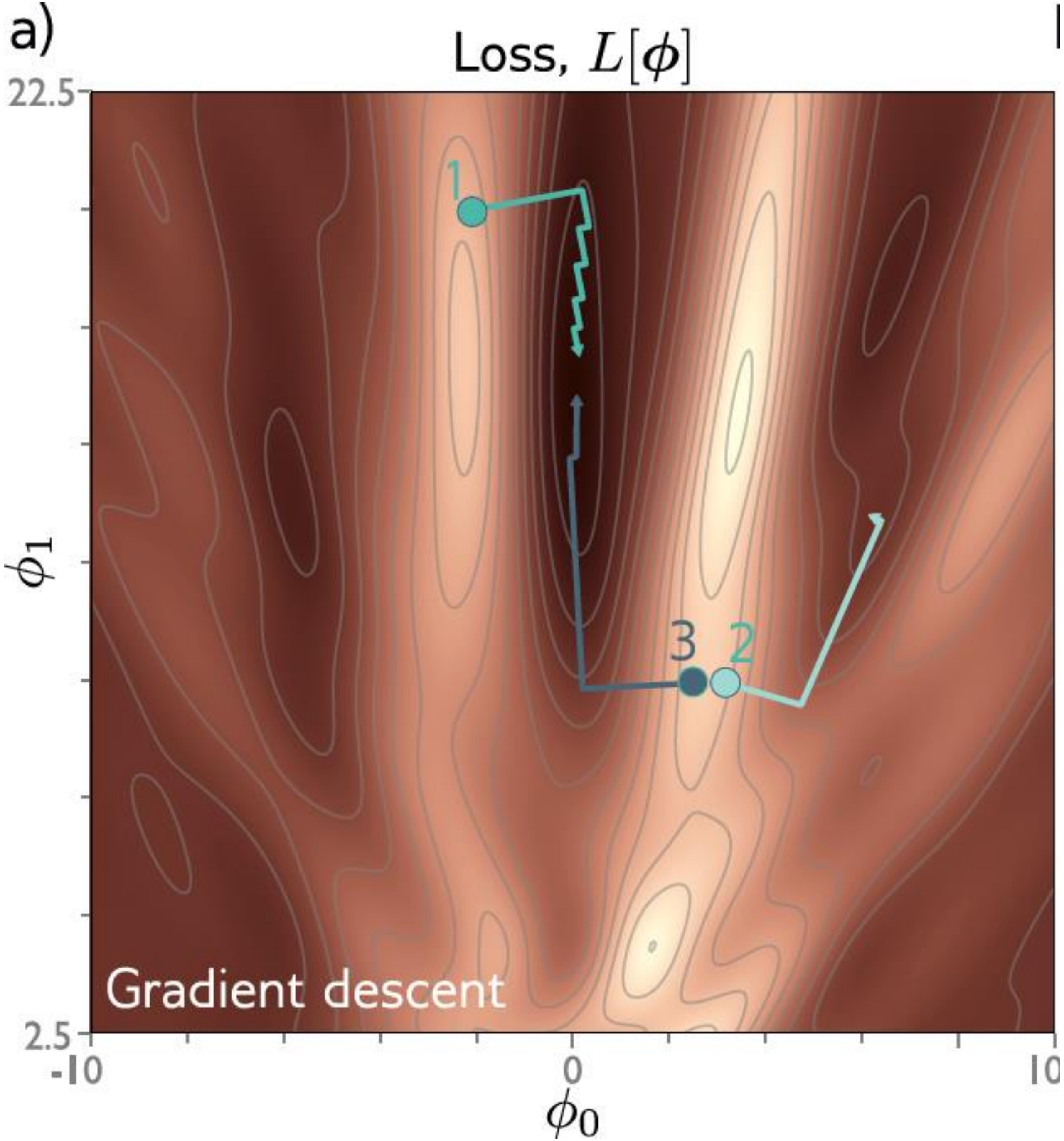

IDEA: add noise, save computation

- 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

Batches and Epochs
(Ex. 30 sample dataset, batch size 5)

Data Indices [0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29]

Permute [27 15 23 17 8 9 28 24 12 0 4 16 5 13 11 22 1 2 25 3 21 26 18 29 20 7 10 14 19 6]

Batch Size 5

30/5 = 6 batches per epoch

```
Epoch # 0-----------
Step 0, Batch # 0, Batch Range [0 1 2 3 4], Batch index: [27 15 23 17 8]
Step 1, Batch # 1, Batch Range [5 6 7 8 9], Batch index: [ 9 28 24 12 0]
Step 2, Batch # 2, Batch Range [10 11 12 13 14], Batch index: [ 4 16 5 13 11]
Step 3, Batch # 3, Batch Range [15 16 17 18 19], Batch index: [22 1 2 25 3]
Step 4, Batch # 4, Batch Range [20 21 22 23 24], Batch index: [21 26 18 29 20]
Step 5, Batch # 5, Batch Range [25 26 27 28 29], Batch index: [ 7 10 14 19 6]
Epoch # 1-----------
Step 6, Batch # 0, Batch Range [0 1 2 3 4], Batch index: [27 15 23 17 8]
Step 7, Batch # 1, Batch Range [5 6 7 8 9], Batch index: [ 9 28 24 12 0]
Step 8, Batch # 2, Batch Range [10 11 12 13 14], Batch index: [ 4 16 5 13 11]
Step 9, Batch # 3, Batch Range [15 16 17 18 19], Batch index: [22 1 2 25 3]

...
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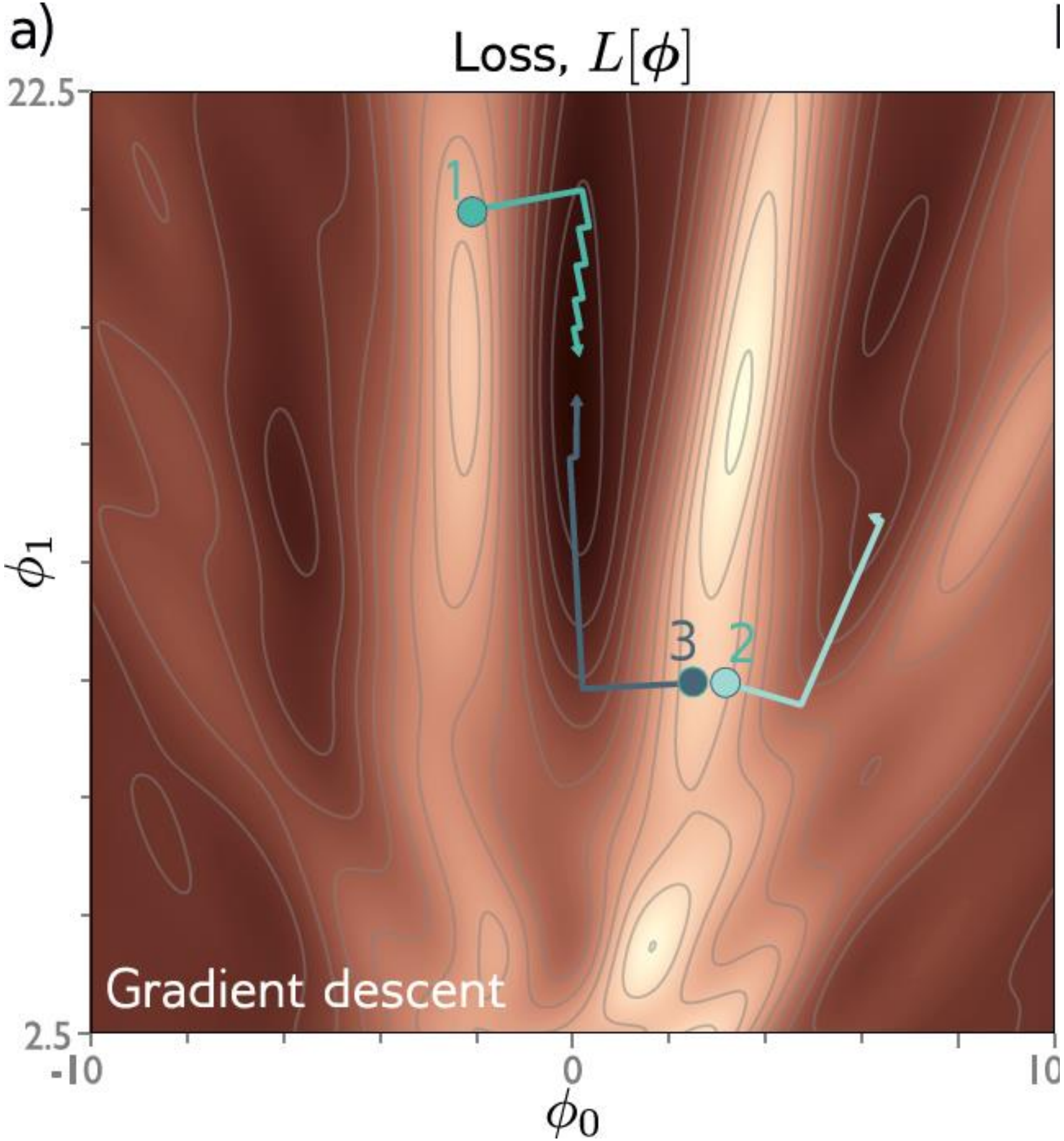


Stochastic gradient descent

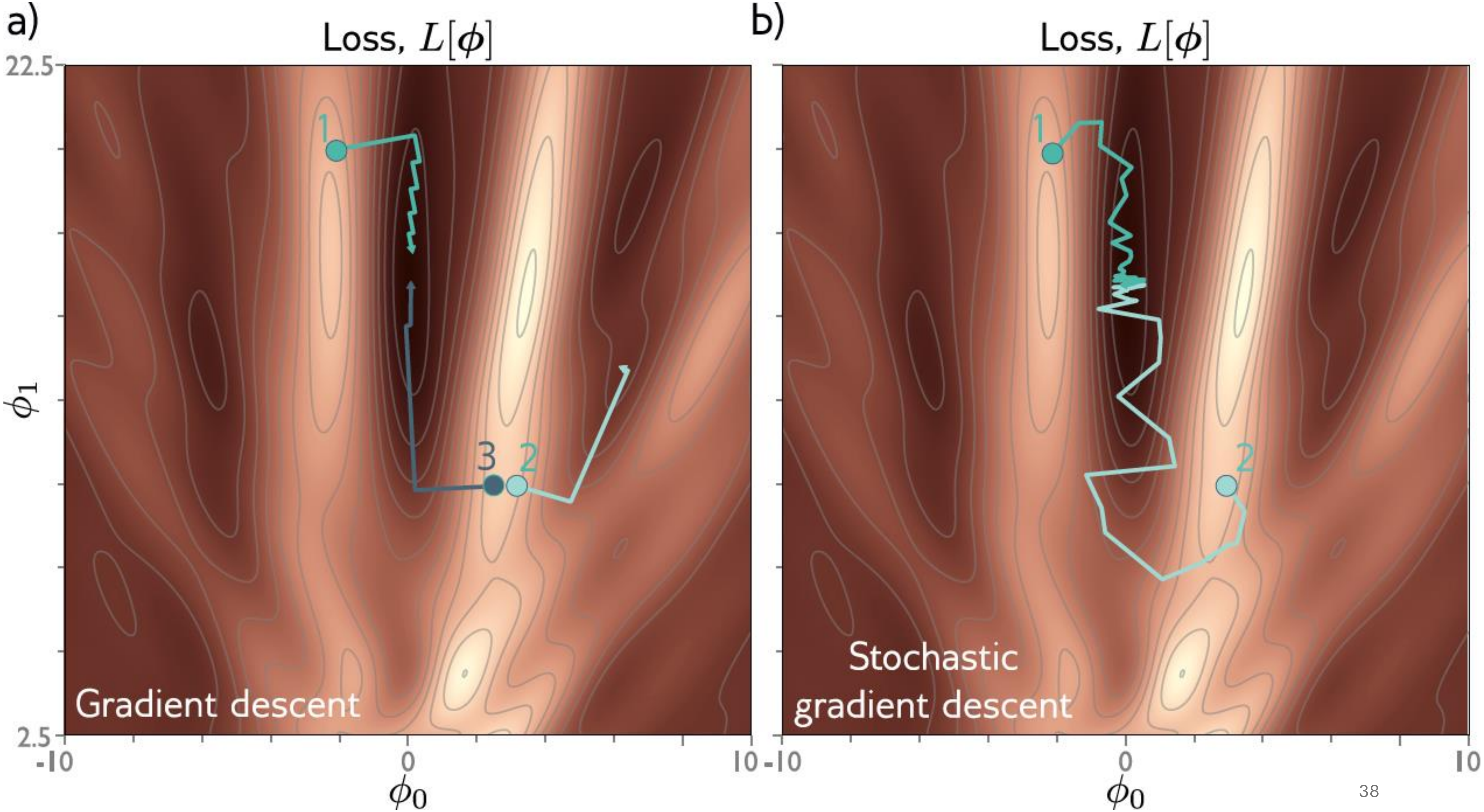
Before (full batch descent)

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

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

Properties of SGD

- Can escape from local minima
- Adds noise, but still sensible updates as based on part of data
- Still 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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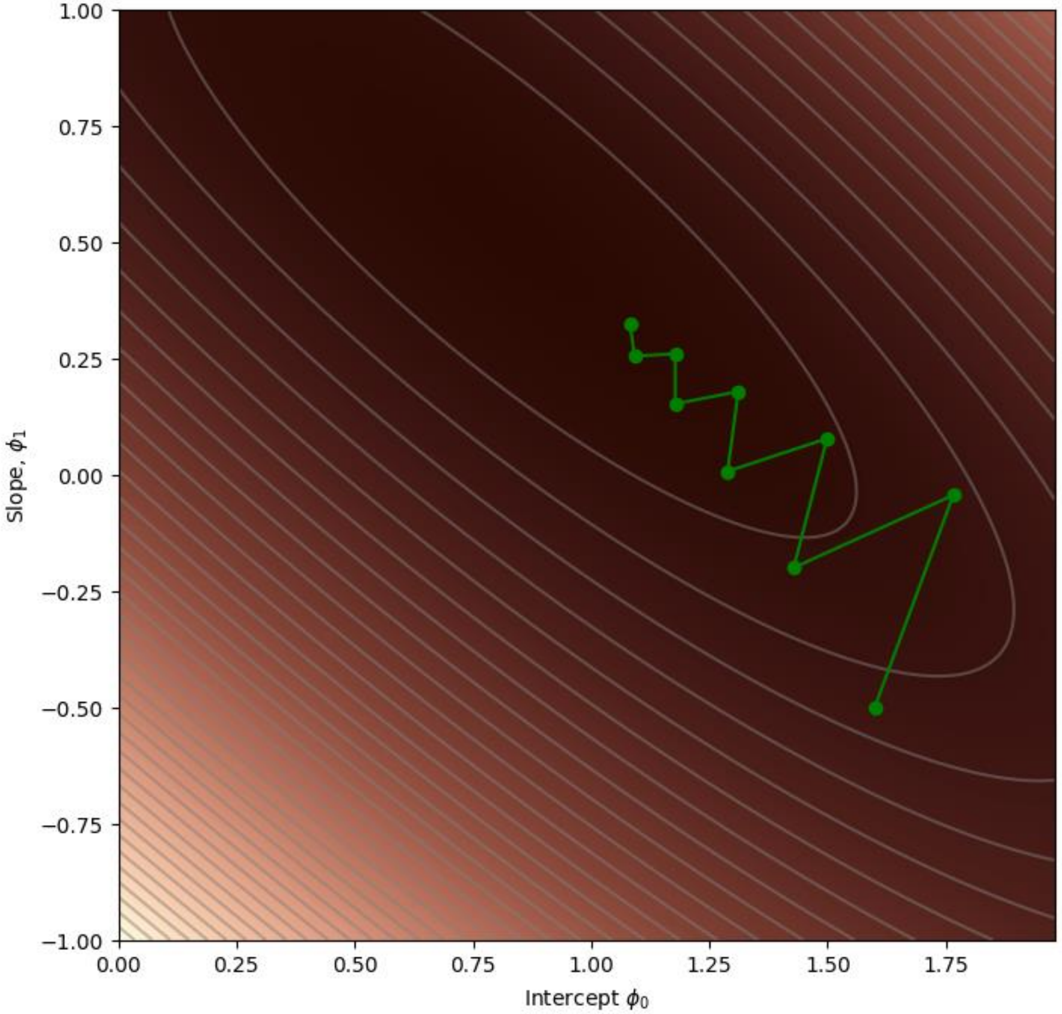
Simple Gradient Descent



Think of analogy of a ball rolling down a hill.

Would it follow path like on the left?

Why/Why not? What’s missing?

Momentum

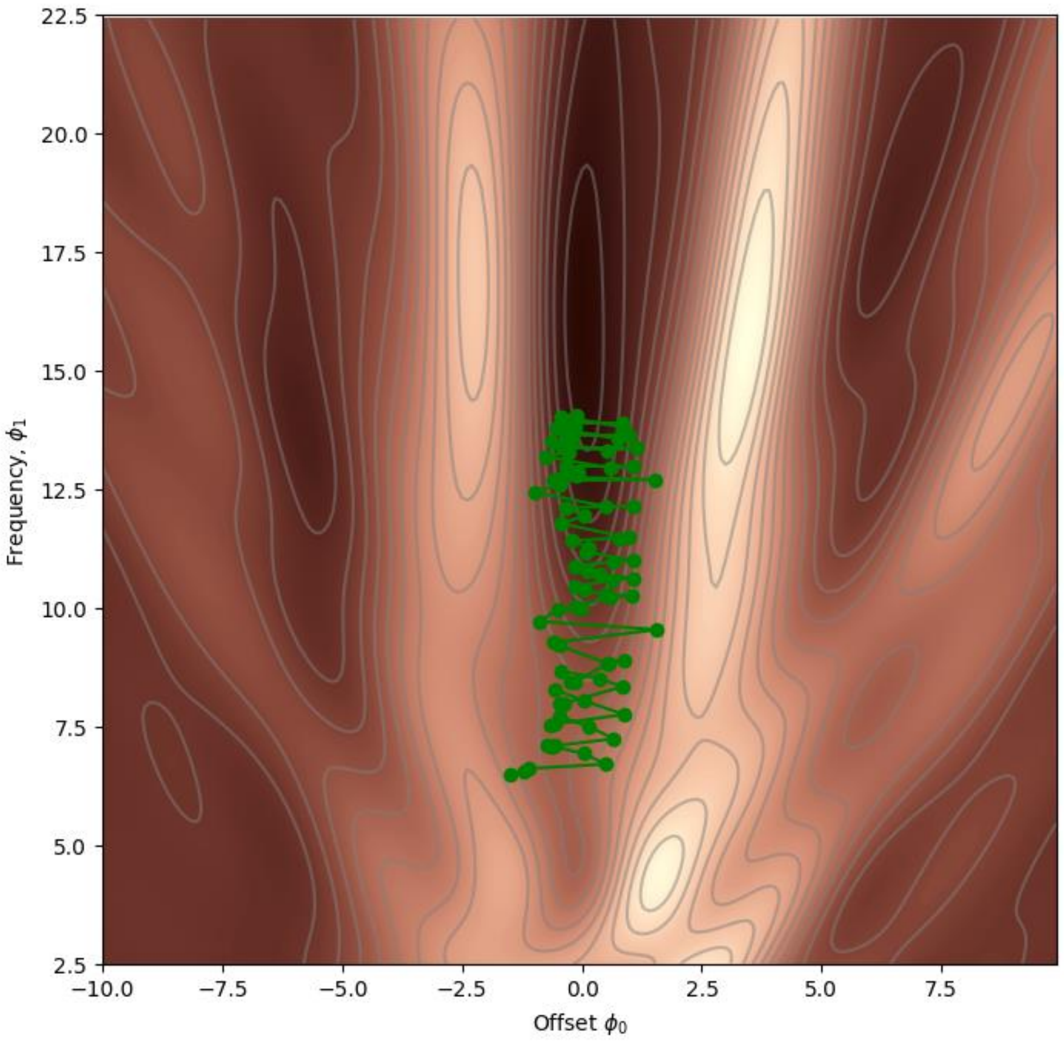
- Weighted sum of this gradient and previous gradient
- Not only influenced by gradient
- Changes more slowly over time

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

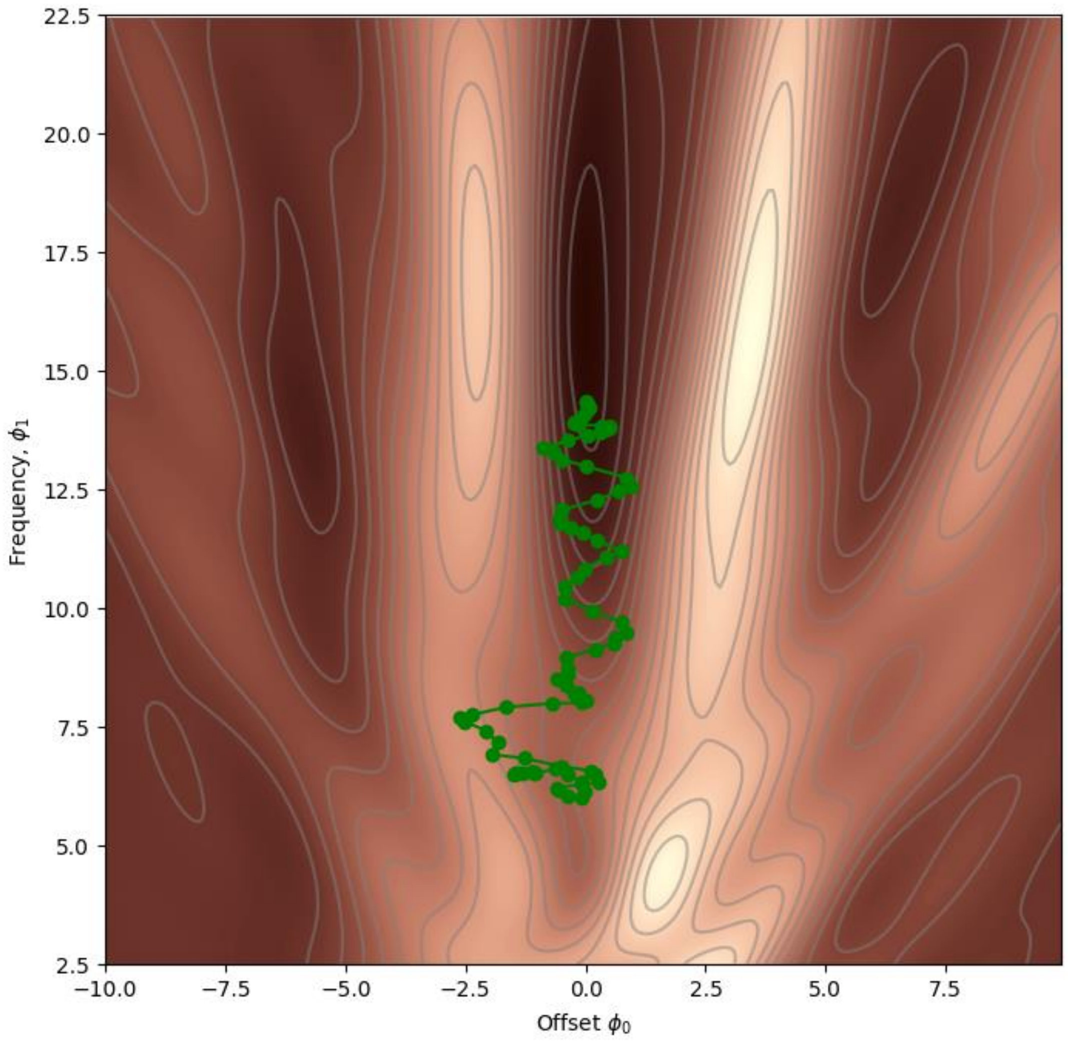
$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_{t+1}$$

Still in batches.

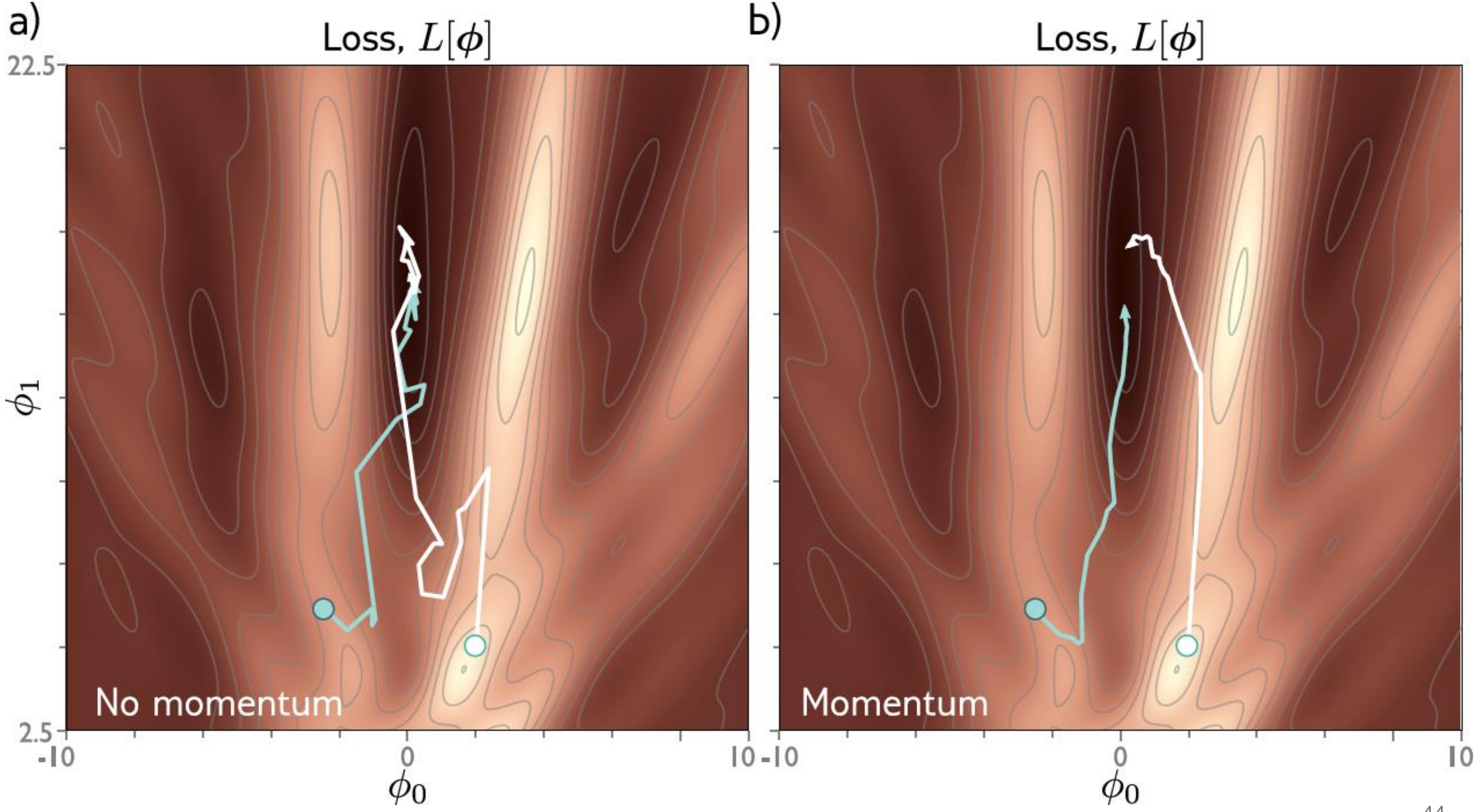
Without and With Momentum



Without Momentum, Loss = 1.31



With Momentum, Loss = 0.96


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

Nesterov accelerated momentum

- Momentum smooths out gradient of current location

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

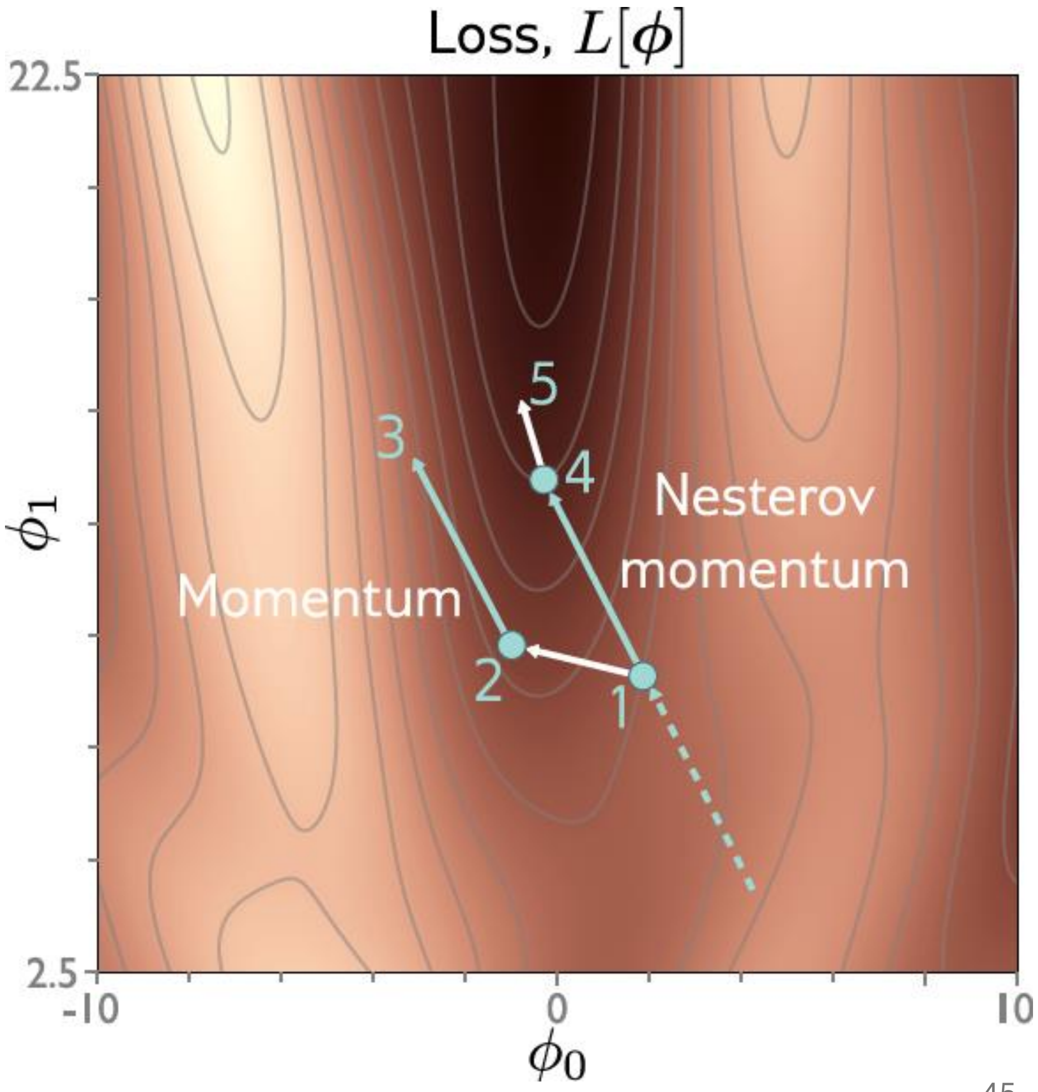
$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_{t+1}$$

- Alternative, smooth out gradient of where we think we will be!

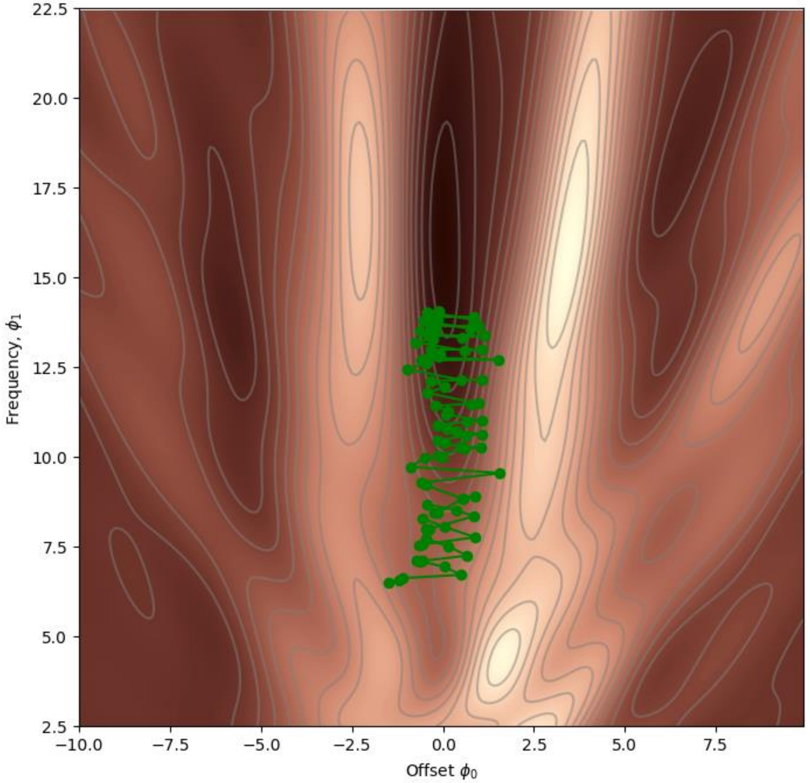
$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta) \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_t]}{\partial \boldsymbol{\phi}}$$

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

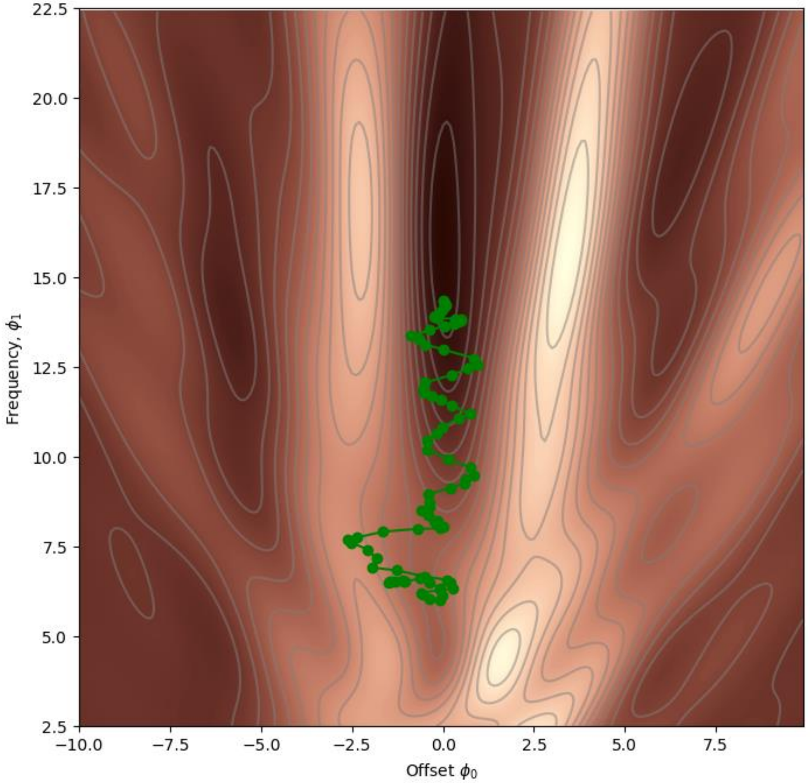
Still in batches.



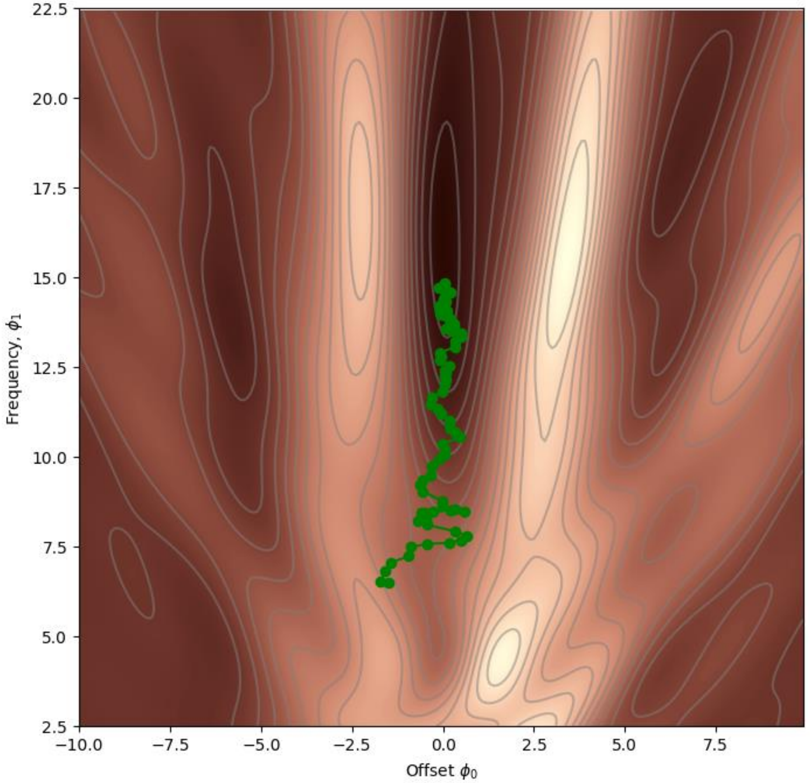
Nesterov Momentum



Without Momentum, Loss = 1.31



With Momentum, Loss = 0.96



Nesterov Momentum, Loss = 0.80

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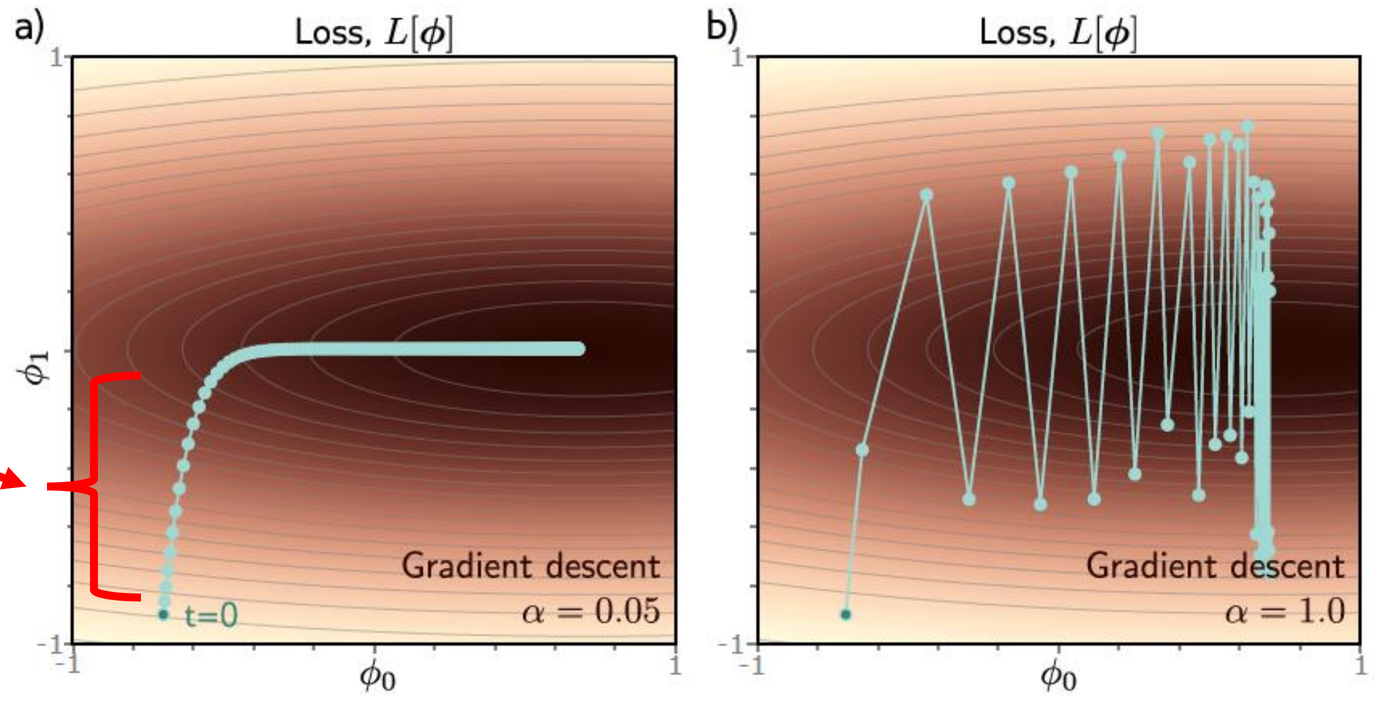
The challenge with fixed step sizes

Moves quickly in one dimension but slowly in the other.



Too small and it will converge slowly, but eventually get there.

Too big and it will move quickly but might bounce around minimum or away.

Solution Part 1: Unit Vector Gradients

- Measure gradient $\mathbf{m}_{t+1}$ and squared magnitude of gradient $\mathbf{v}_{t+1}$

$$m_{t+1} \leftarrow \frac{\partial L[\phi_t]}{\partial \phi}$$

$$v_{t+1} \leftarrow \left|\frac{\partial L[\phi_t]}{\partial \phi}\right|^2$$

- Normalize:

$$\phi_{t+1} \leftarrow \phi_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$

α is the learning rate
ϵ is a small constant to prevent div by 0
Square, sqrt and div are all pointwise

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ϵ is a small constant to prevent div by 0
Square, sqrt and div are all pointwise

Dividing by the magnitude, so normalized to unit vector.

Solution Part 1: Unit Vector gradients

- Measure mean and pointwise squared gradient

$$m_{t+1} \leftarrow \frac{\partial L[\phi_t]}{\partial \phi}$$

$$v_{t+1} \leftarrow \left|\frac{\partial L[\phi_t]}{\partial \phi}\right|^2$$

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

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

$$v_{t+1} = 3^2 + (-2)^2 + 5^2 = 38$$

- Normalize:

$$\phi_{t+1} \leftarrow \phi_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$

$$\frac{m_{t+1}}{\sqrt{\boldsymbol{v}_{t+1}} + \text{\textbackslash epsilon}} \approx \begin{bmatrix} +0.49 \\ -0.32 \\ +0.81 \end{bmatrix}$$

Large gradient components suppress other gradient components!

Solution Part 2: Normalized gradients

- Measure gradient $\mathbf{m}_{t+1}$ and pointwise squared gradient $\mathbf{v}_{t+1}$

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

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

- Normalize:

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

α is the learning rate
ϵ is a small constant to prevent div by 0
Square, sqrt and div are all pointwise

Solution Part 2: Normalized gradients

- Measure gradient $\mathbf{m}_{t+1}$ and pointwise squared gradient $\mathbf{v}_{t+1}$

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

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

- Normalize:

$$\phi_{t+1} \leftarrow \phi_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$

α is the learning rate
ϵ is a small constant to prevent div by 0
Square, sqrt and div are all pointwise

Dividing by the positive root, so normalized to 1 and all that is left is the sign.

Solution Part 2: Normalized gradients

- Measure mean and pointwise squared gradient

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

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

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

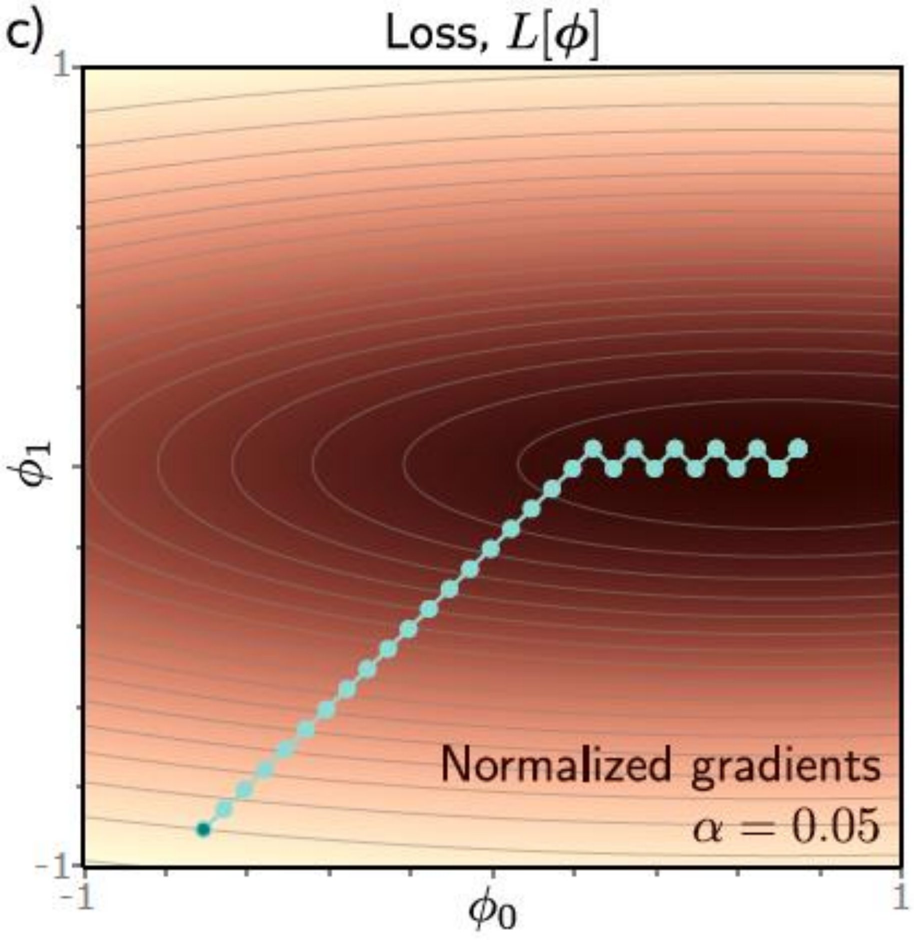
$$\mathbf{v}_{t+1} = \begin{bmatrix} 9.0 \\ 4.0 \\ 25.0 \end{bmatrix}$$

- Normalize:

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

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

Solution Part 2: Normalized gradients



- algorithm moves downhill a fixed distance α along each coordinate
- makes good progress in both directions
- but will not converge unless it happens to land exactly at the minimum

Adaptive moment estimation (Adam)

- Compute mean and pointwise squared gradients *with momentum*

$$\begin{cases} \mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta)\dfrac{\partial L[\phi_t]}{\partial \phi} \\ \mathbf{v}_{t+1} \leftarrow \gamma \cdot \mathbf{v}_t + (1-\gamma)\left(\dfrac{\partial L[\phi_t]}{\partial \phi}\right)^2 \end{cases}$$

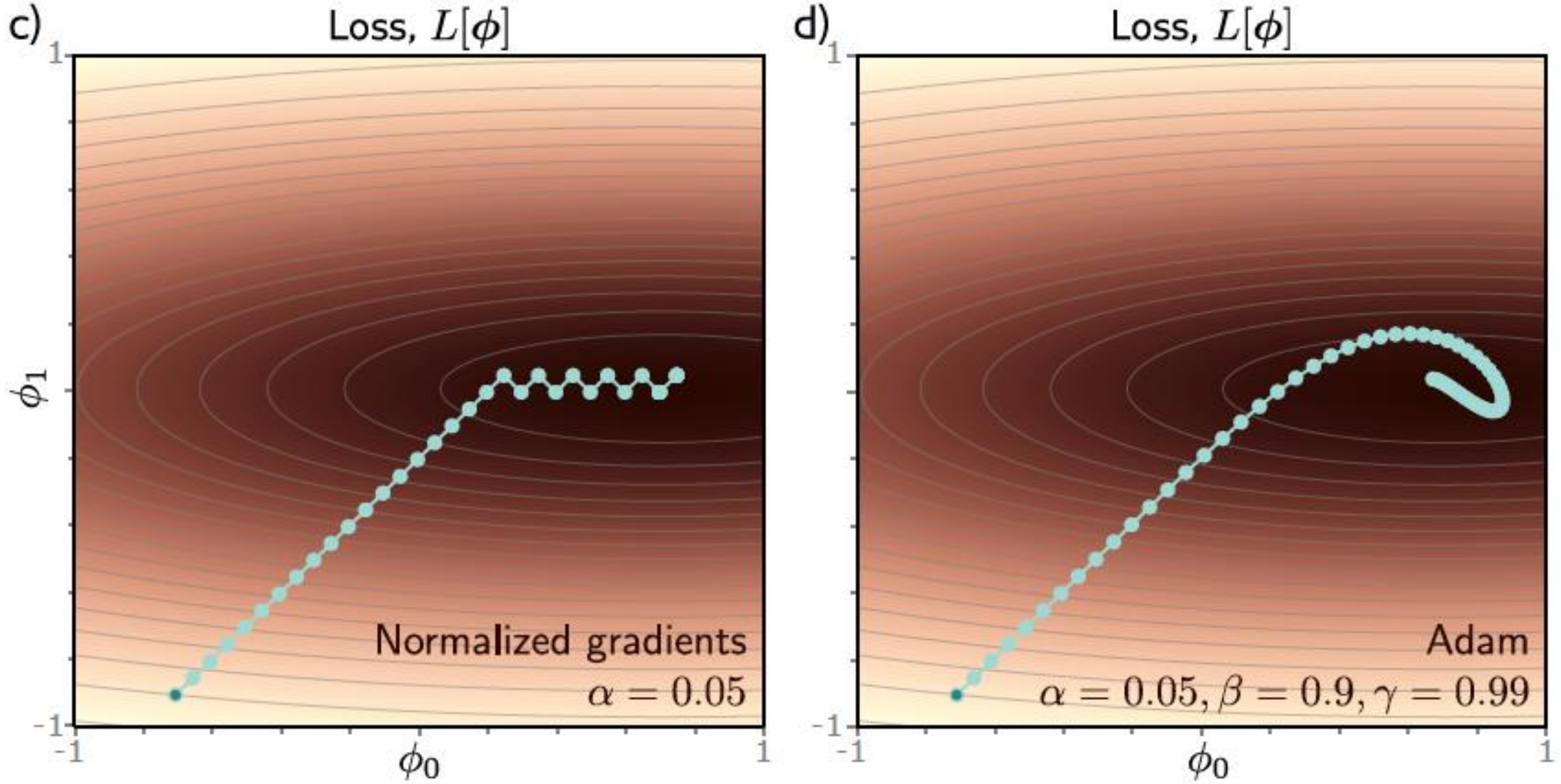
- Boost momentum near start of the sequence since they are initialized to zero

$$\begin{cases} \tilde{\mathbf{m}}_{t+1} \leftarrow \dfrac{\mathbf{m}_{t+1}}{1-\beta^{t+1}} \\ \tilde{\mathbf{v}}_{t+1} \leftarrow \dfrac{\mathbf{v}_{t+1}}{1-\gamma^{t+1}} \end{cases} \qquad \begin{aligned} \mathbf{m}_{t=0} &= 0 \\ \mathbf{v}_{t=0} &= 0 \end{aligned}$$

- Update the parameters

$$\begin{cases} \phi_{t+1} \leftarrow \phi_t - \alpha \cdot \dfrac{\tilde{\mathbf{m}}_{t+1}}{\sqrt{\tilde{\mathbf{v}}_{t+1}} + \epsilon} \end{cases}$$

Adaptive moment estimation (Adam)



Other advantages of ADAM

- Gradients can diminish or grow deep into networks. ADAM balances out changes across depth of layers.
- Adam is less sensitive to the initial learning rate, so it doesn't need complex learning rate schedules.

Additional Hyperparameters

- Choice of learning algorithm
  - SGD
  - Momentum
  - Nesterov Momentum
  - ADAM
- Learning rate
  - Fixed
  - Schedule
  - Loss dependent
- Momentum Parameters

Recap

- Gradient Descent – Find a minimum for non-convex, complex loss functions
- Stochastic Gradient Descent – Save compute by calculating gradients in batches, which adds some noise to the search
- (Nesterov) Momentum – Add momentum to the gradient updates to smooth out abrupt gradient changes
- ADAM – Correct for inbalance between gradient components while providing some momentum