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

logistic regression = sigmoid(linear(x))

Raise your hand if you encountered any of the following.

- Bad prediction accuracy — not gradual
- learning rate too low
- Loss function improving very slowly
- learning rate too high
- Loss function going up
- NaN or infinity in loss calculations
- NaN in initial loss calculations?

learning rate

initialization

NaN from log(0)

$p = \frac{1}{1+e^{-z}}$

$0 < \frac{1}{1+e^{-z}} < 1$ if z finite (in theory)

in practice, big negative z by float limits

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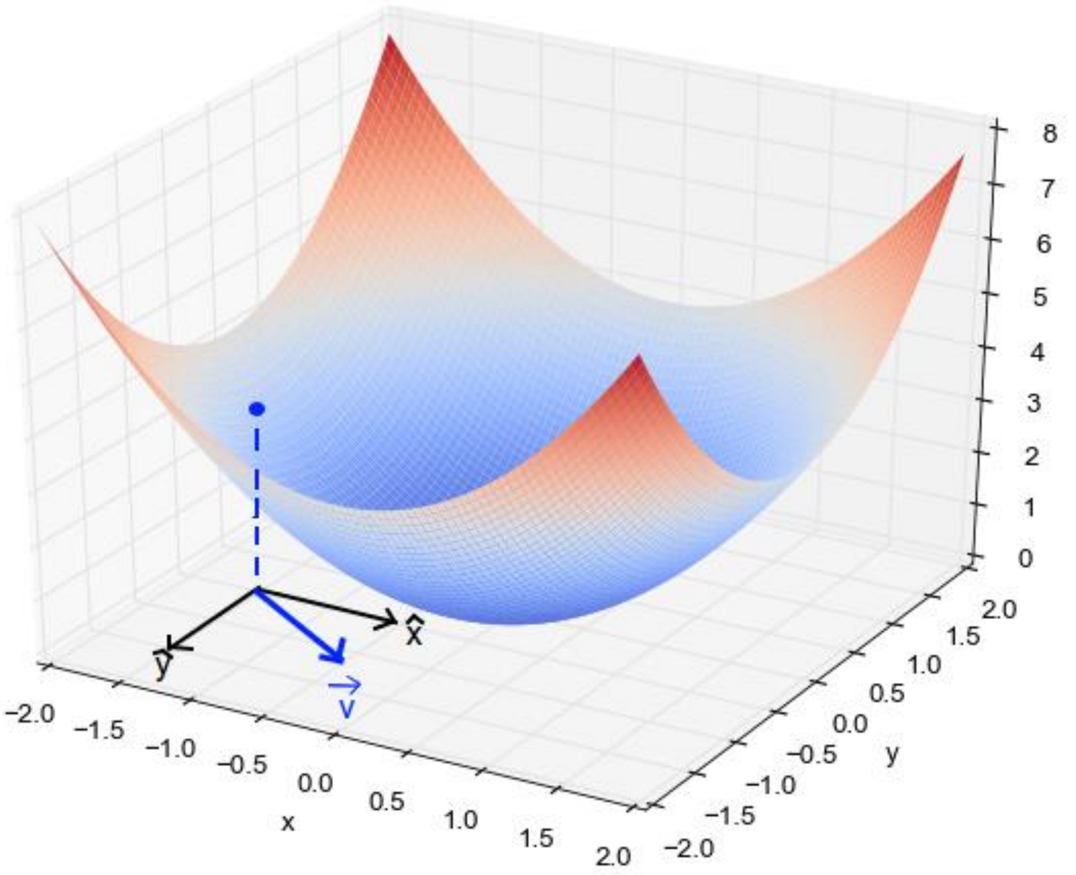
Gradient

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

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:

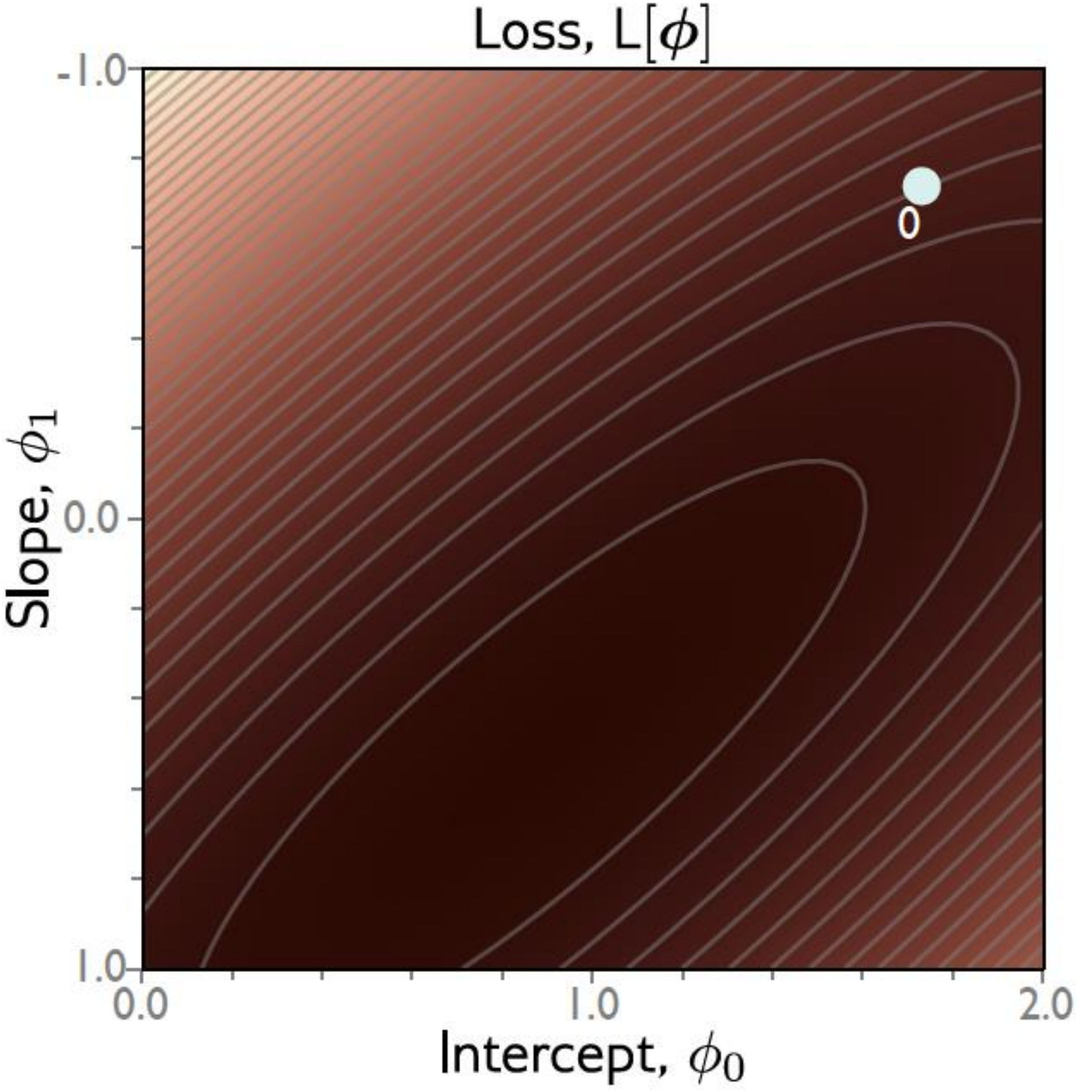
$$\phi \longleftarrow \phi - \alpha \frac{\partial L}{\partial \phi},$$

minus for opposite direction.

α = learning rate.

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

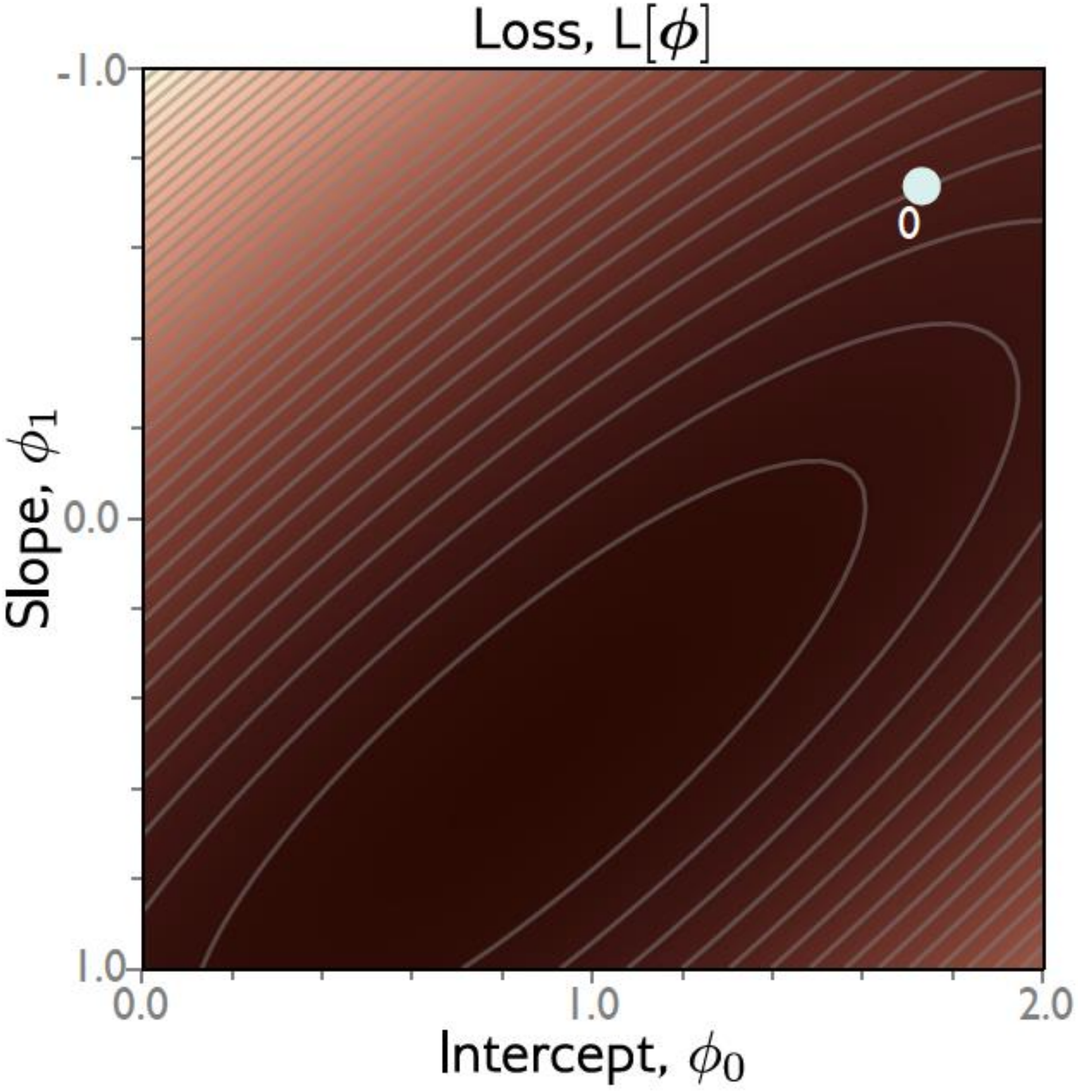
Gradient descent



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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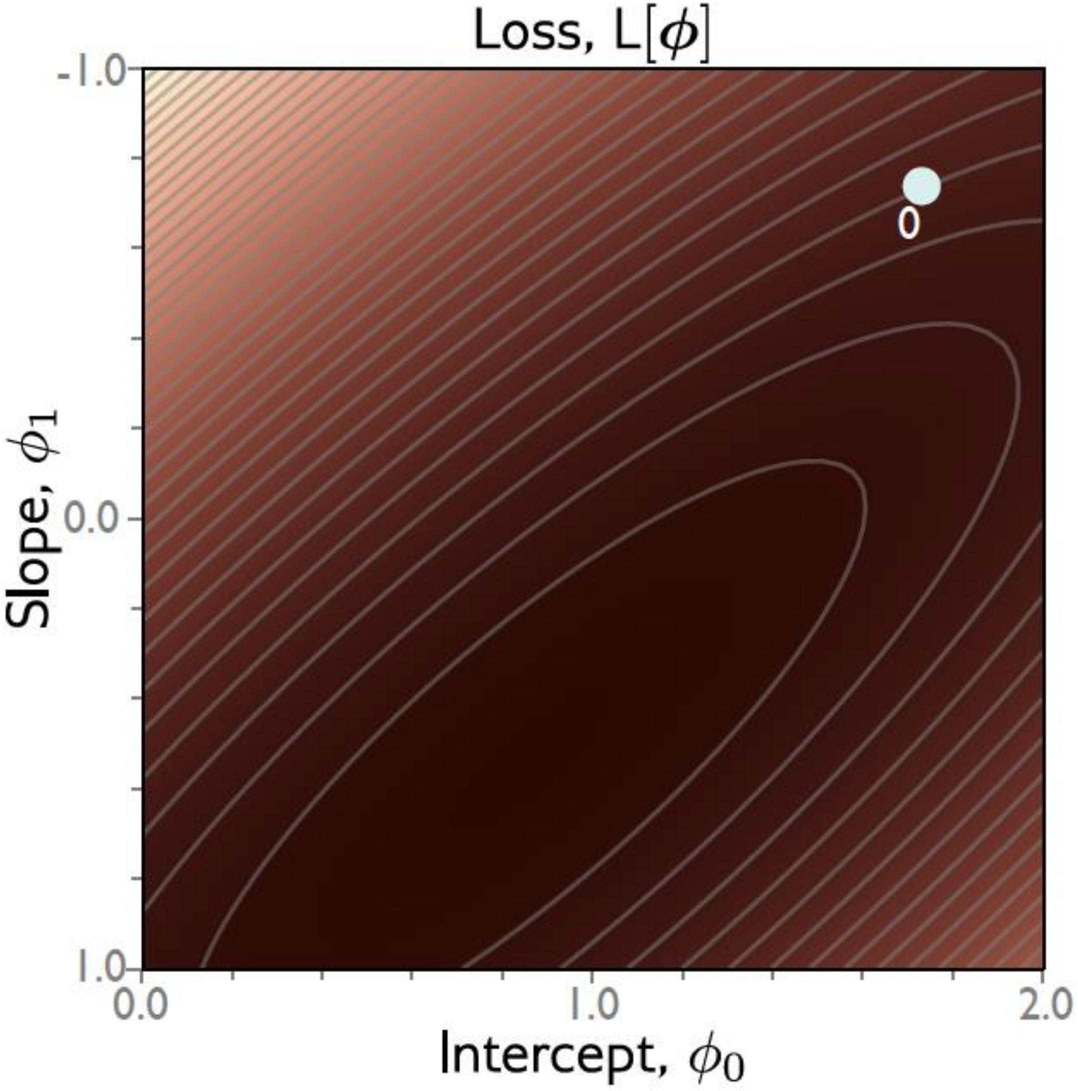
Gradient descent



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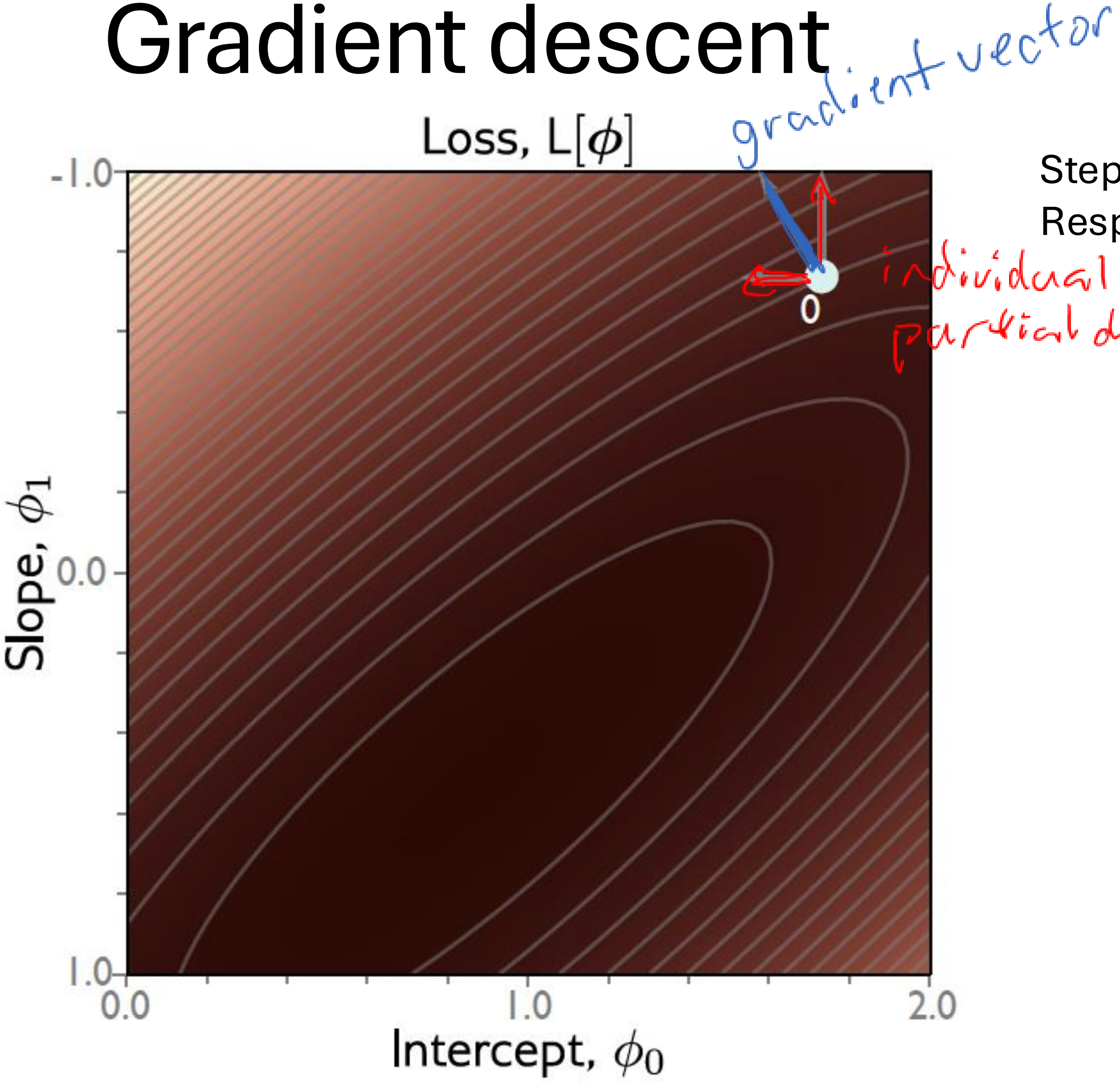
Gradient descent



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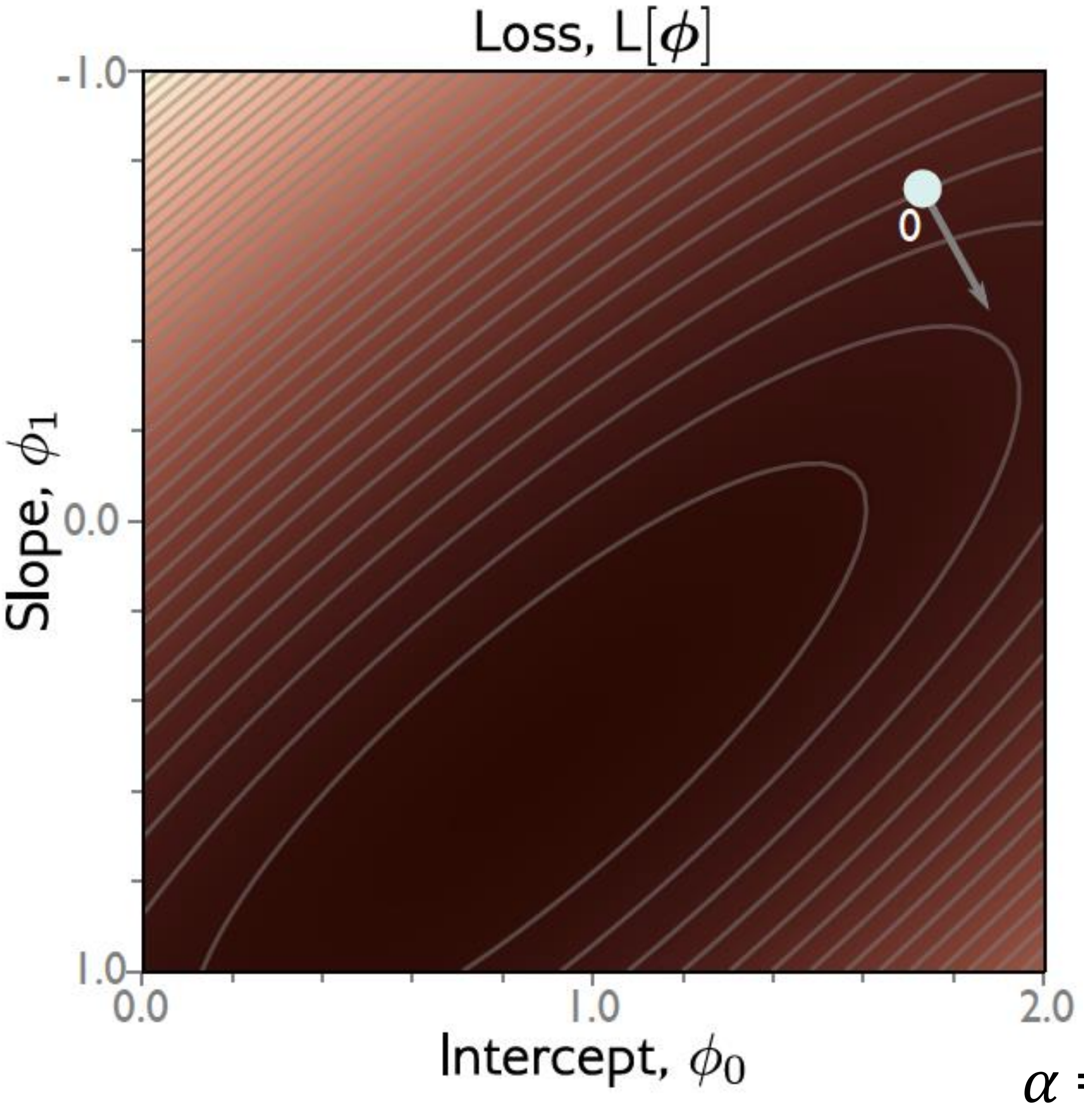
Gradient descent



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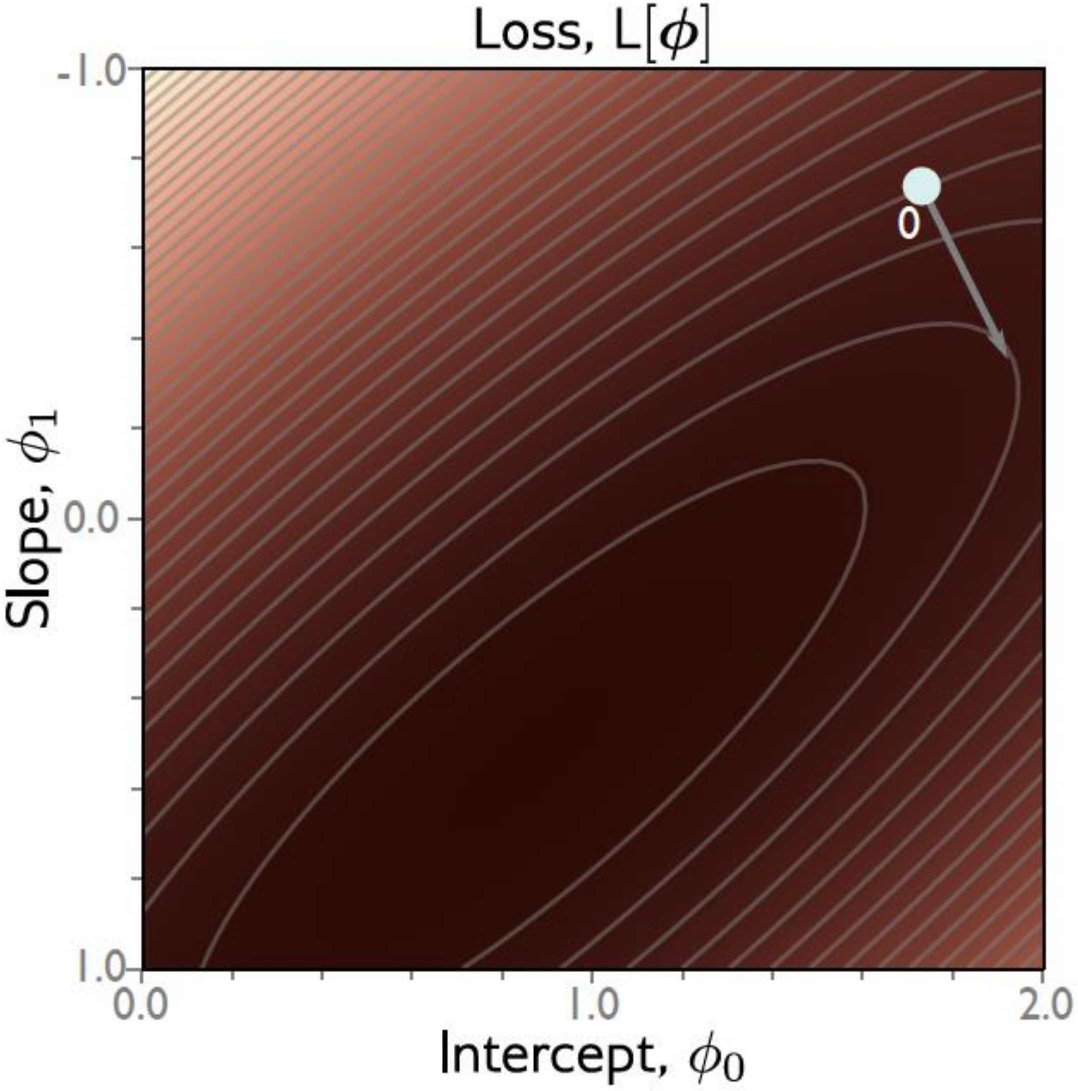
Step 2: Update parameters according to rule

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

α = step size or learning rate if fixed

Gradient descent



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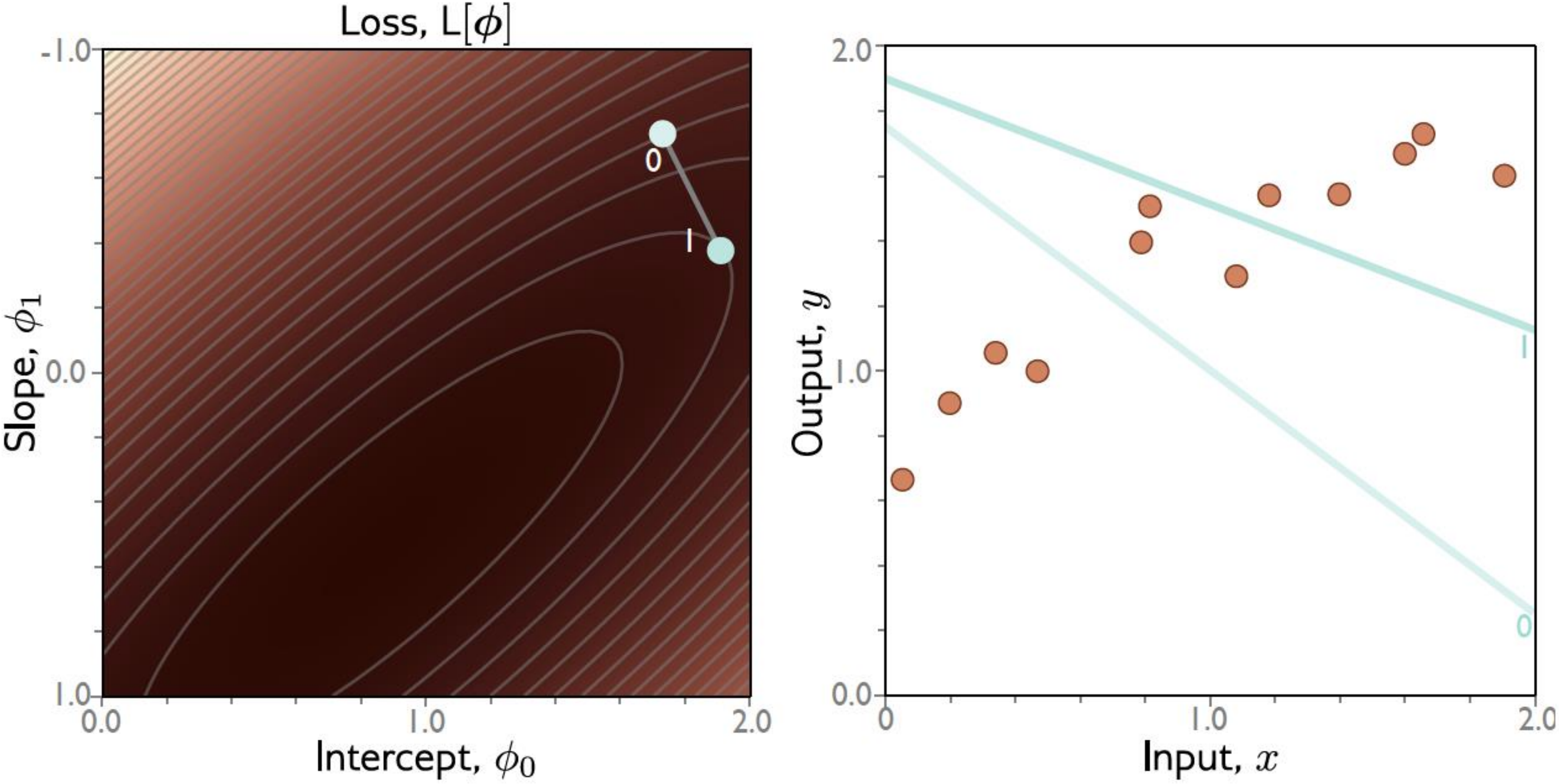
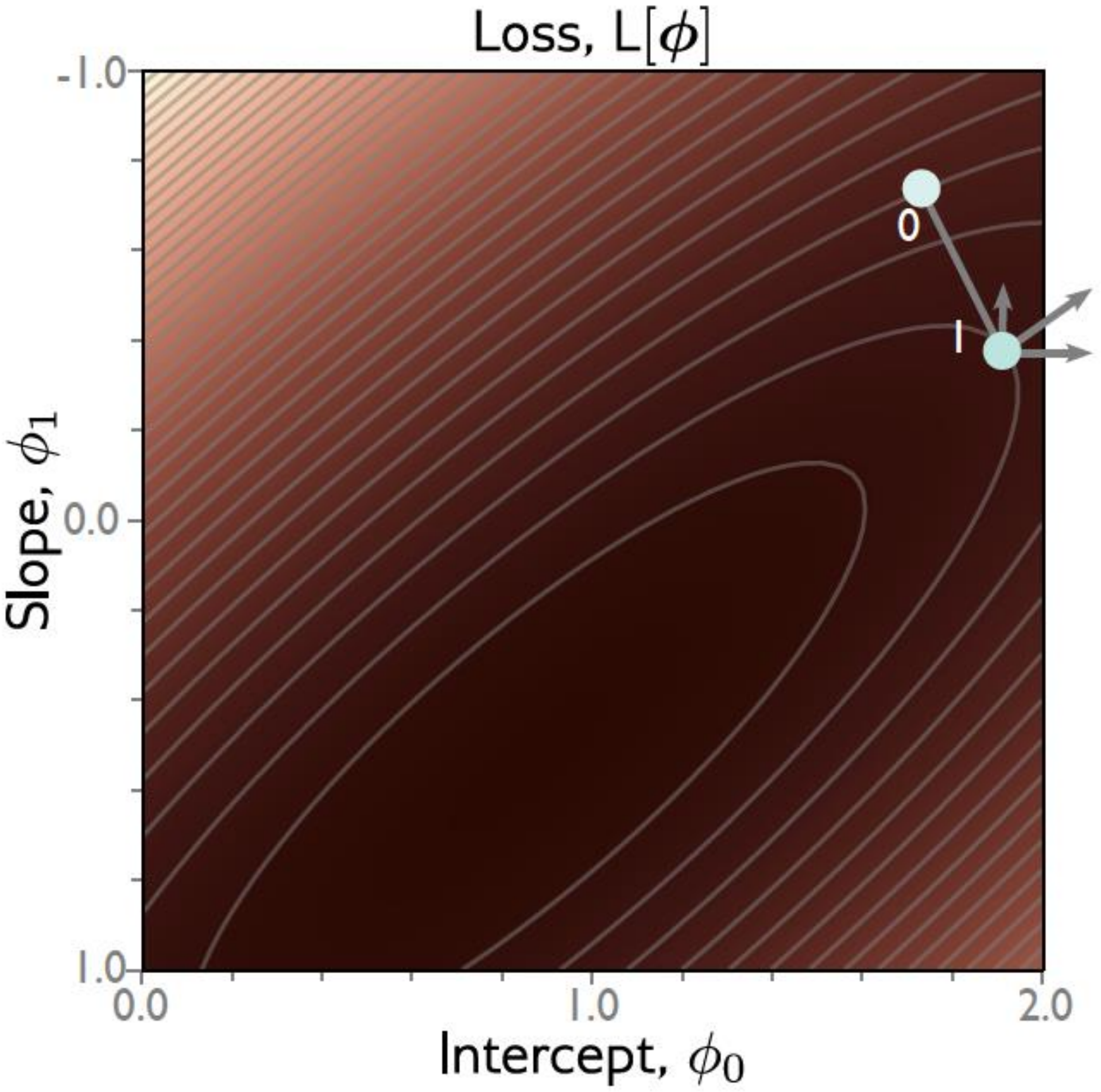
α = step size

Gradient descent



Gradient descent



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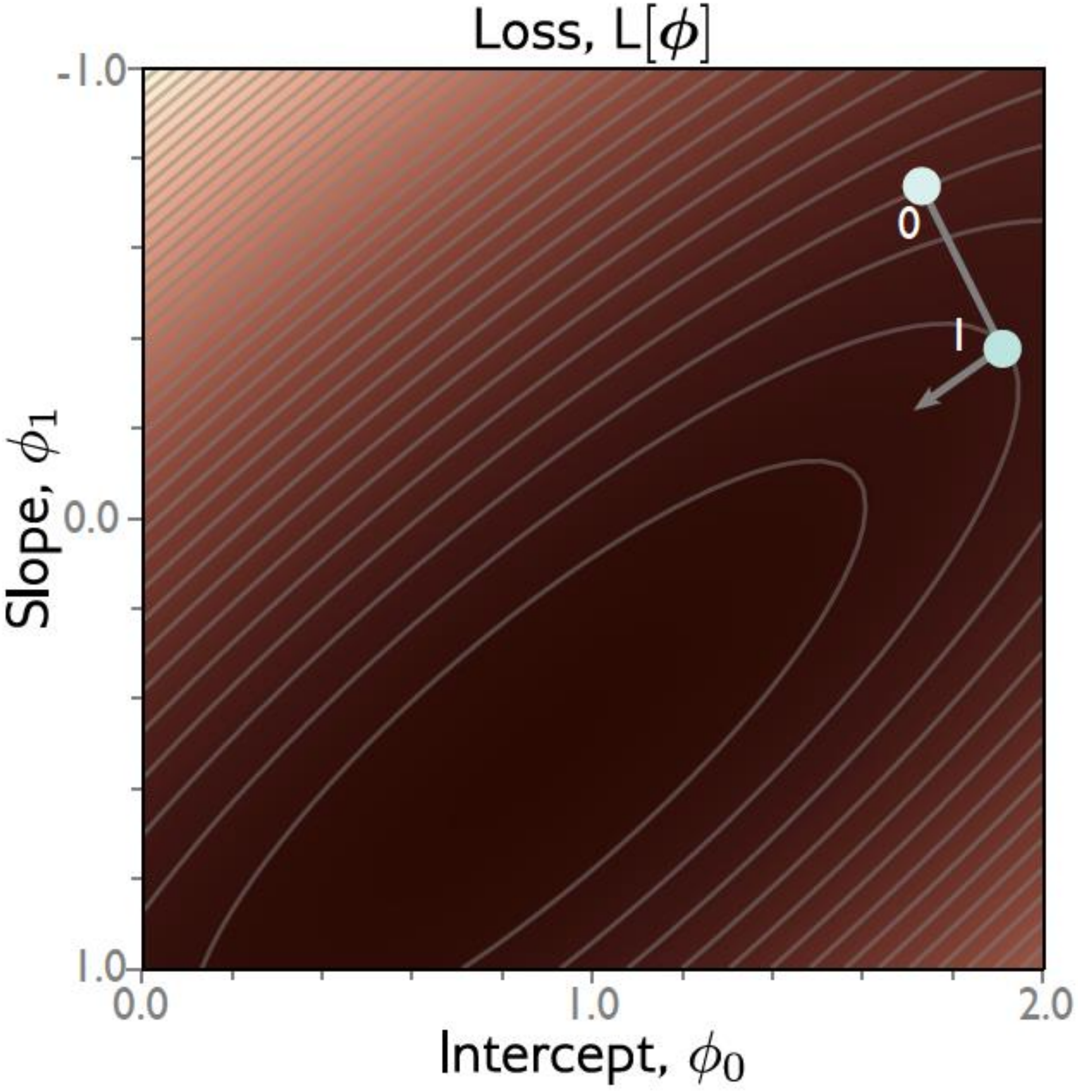

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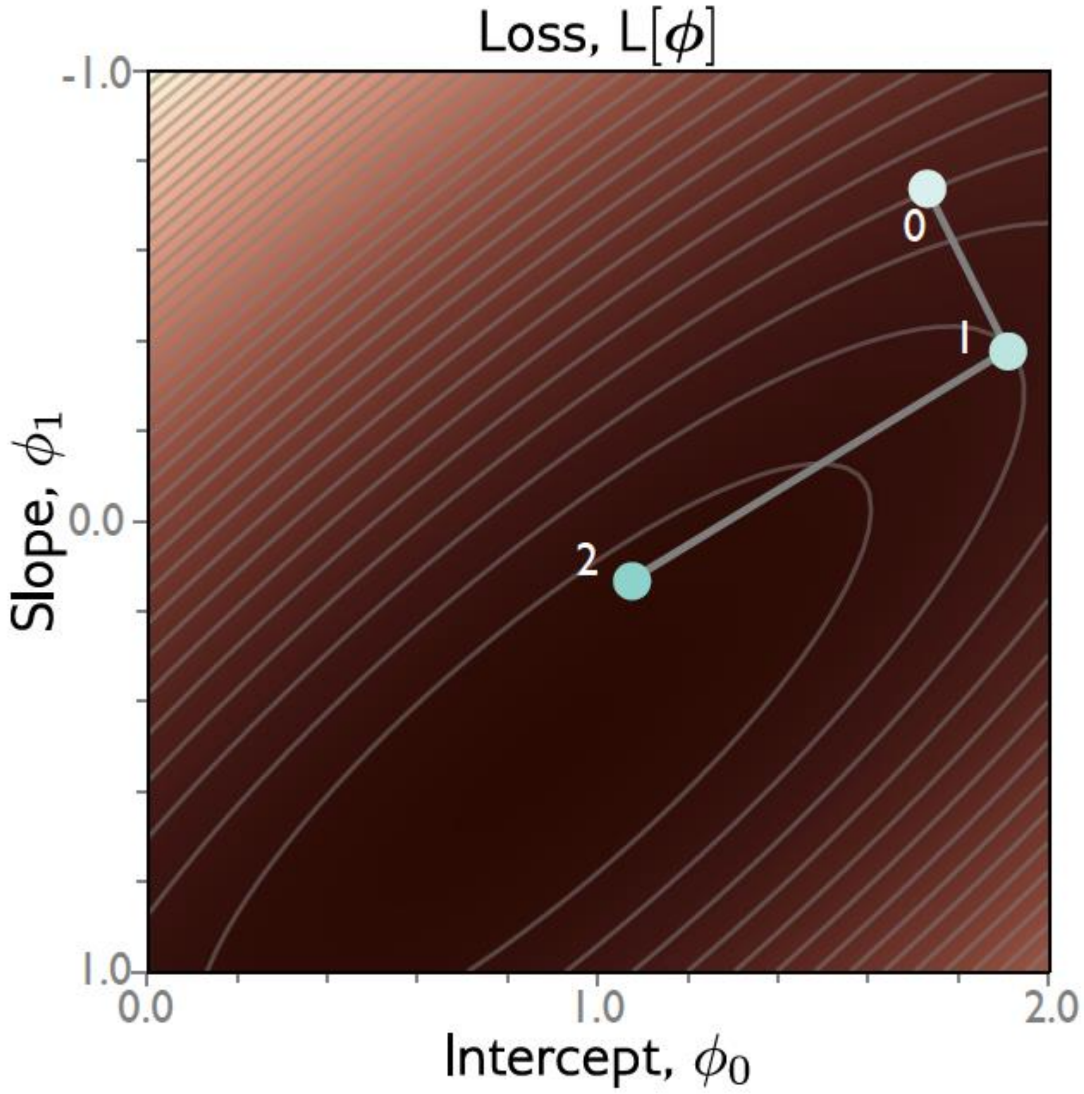
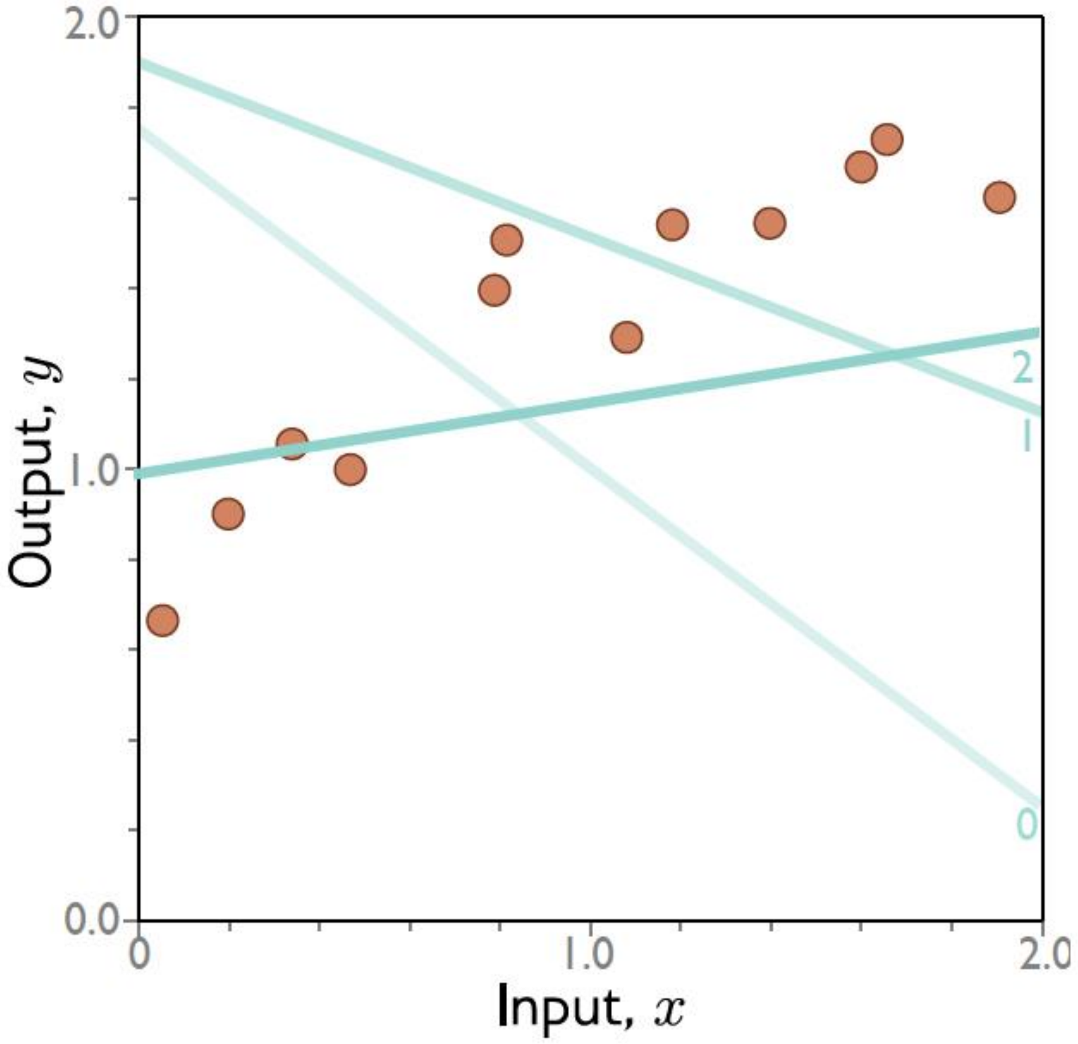
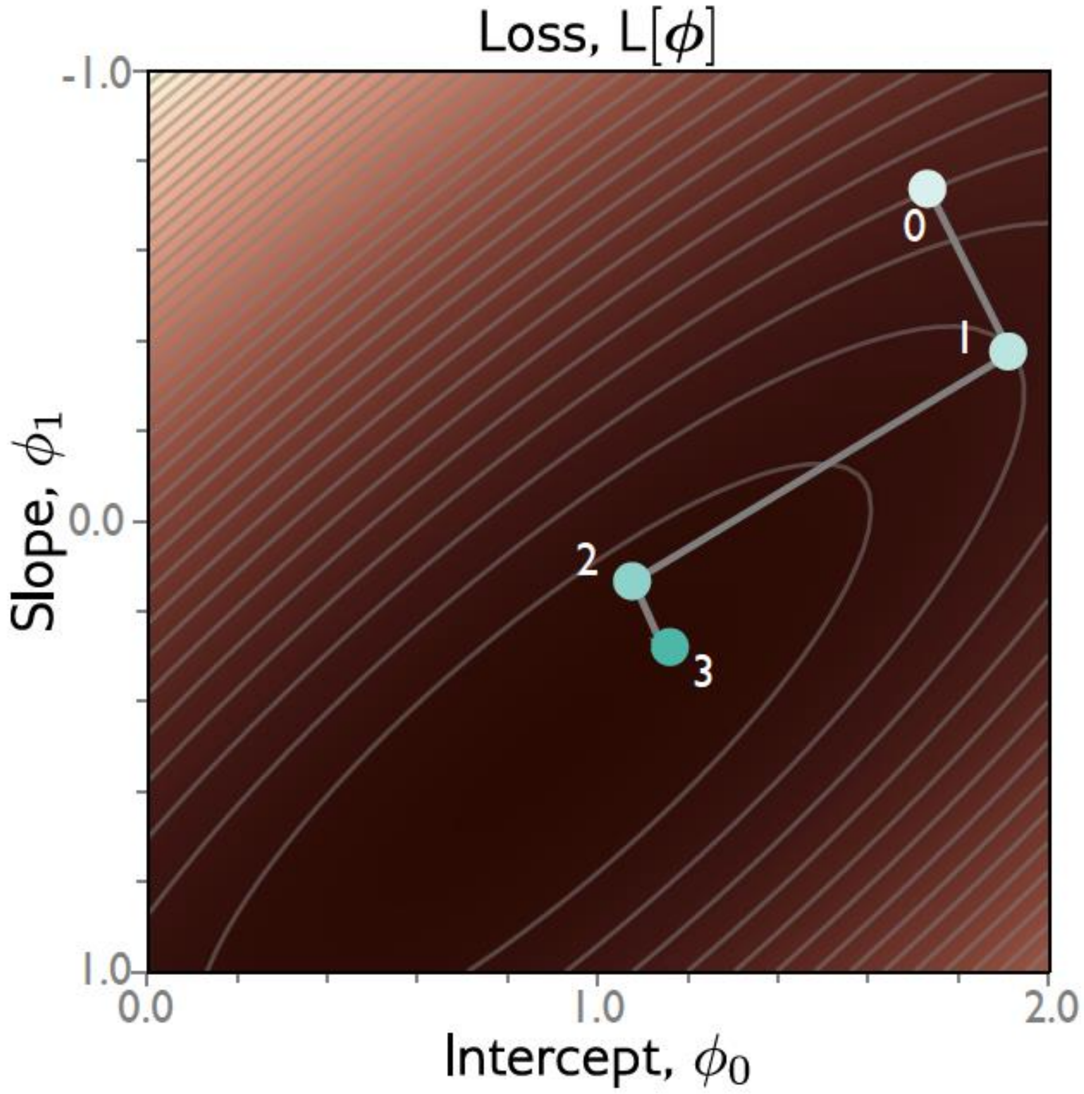
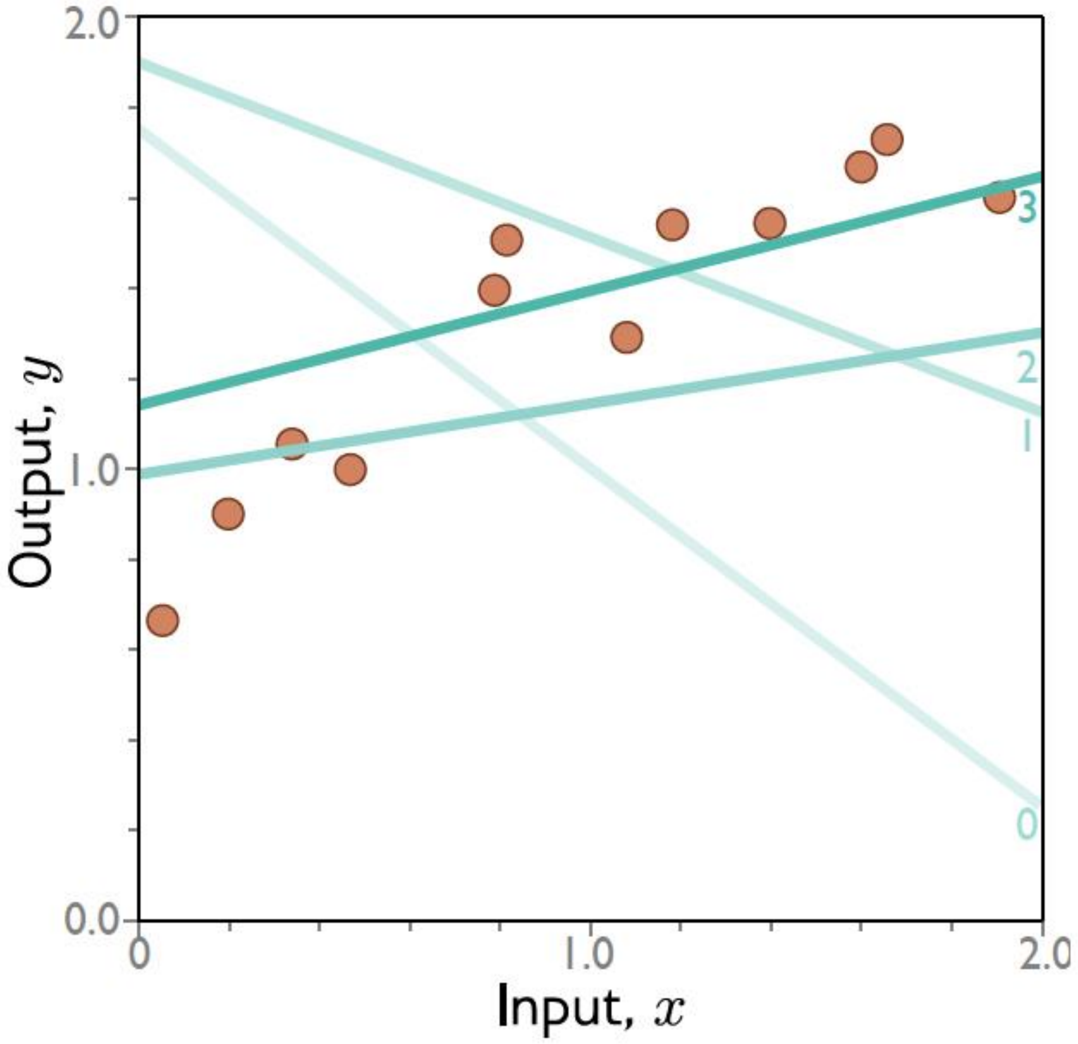
Gradient descent



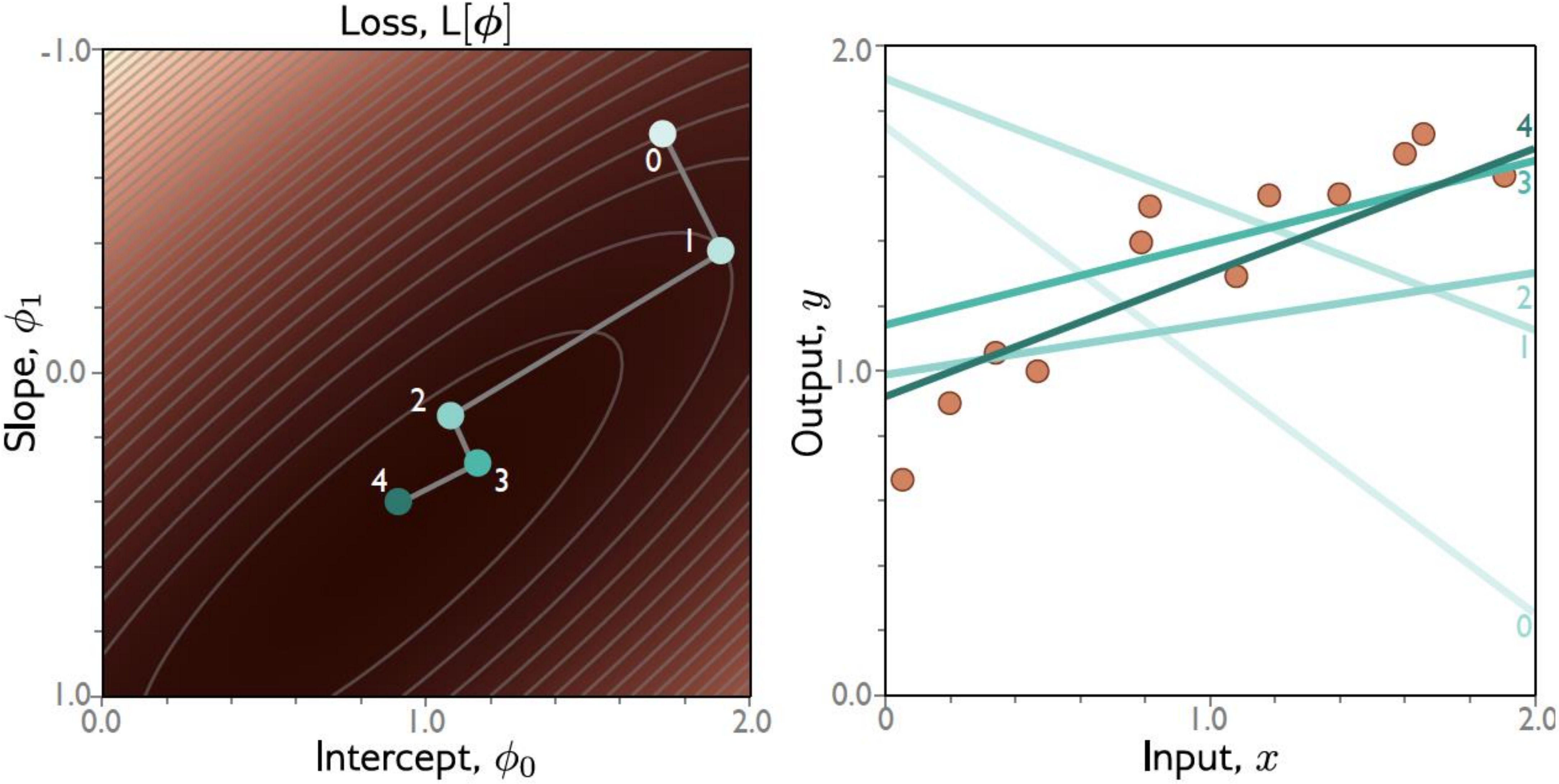


Gradient descent





Gradient descent



The linear model loss function was convex.

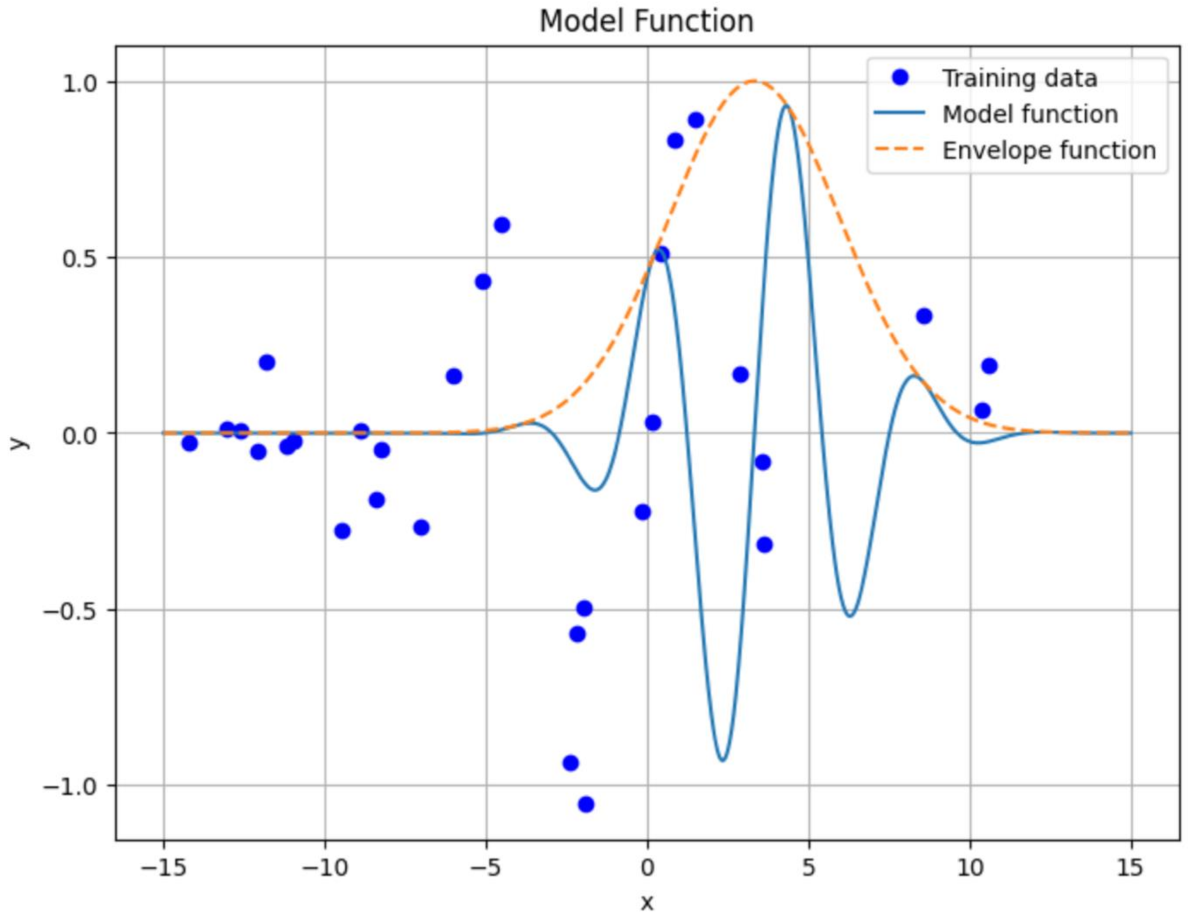
We’ll use a more complex (non-convex) model that we can still visualize in 2D and 3D

➔ Gabor Function

Gabor Model (with Envelope)

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

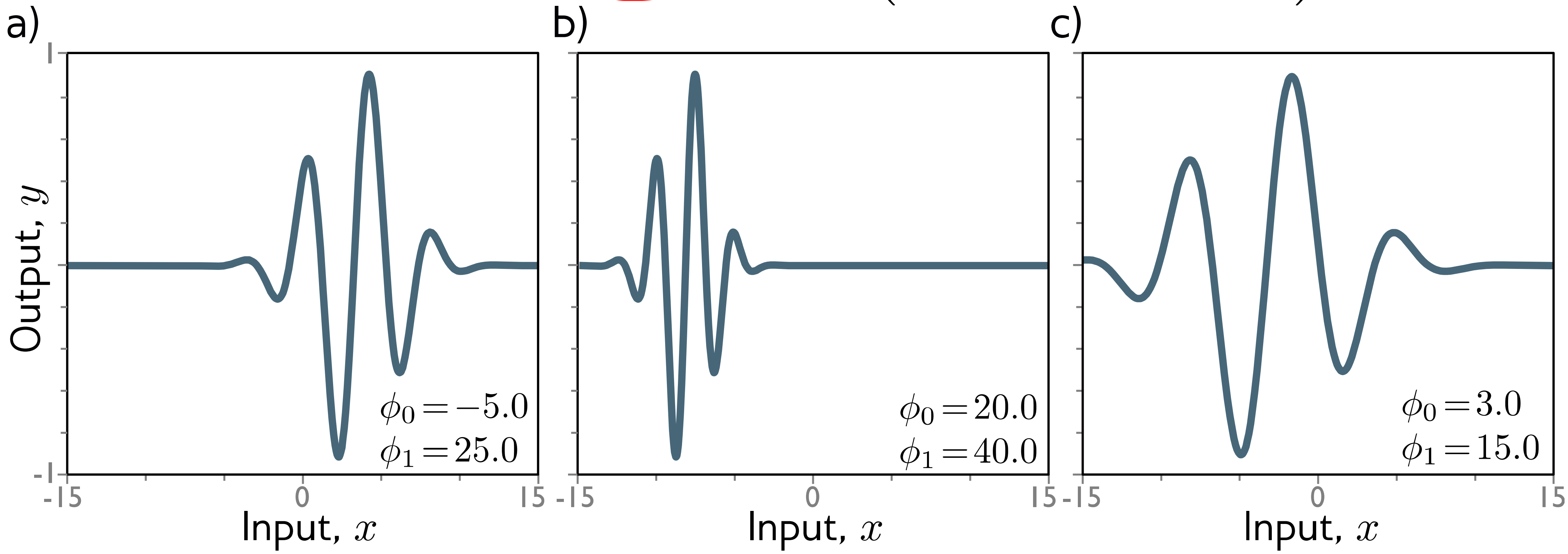
just 2 parameters.



Gabor model

repeated

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

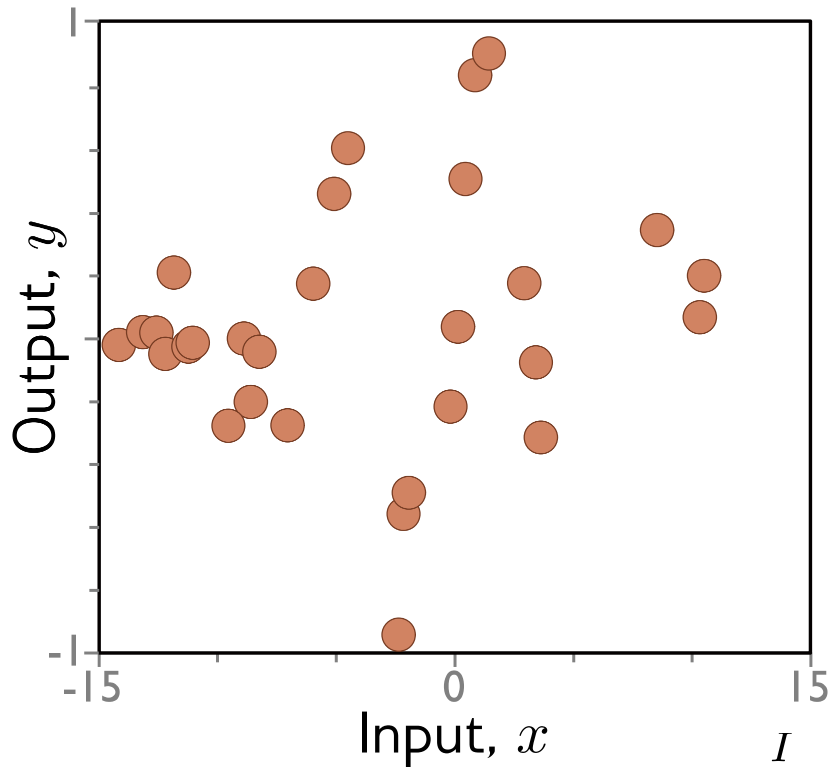


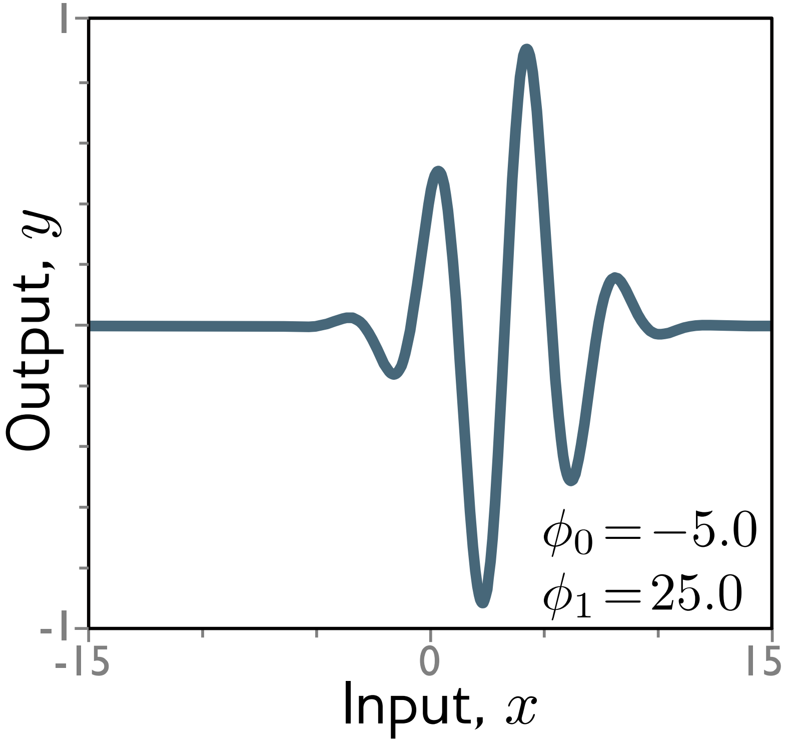
ϕ_0 shifts left and right

ϕ_1 shrinks and expands the sinusoid and envelope

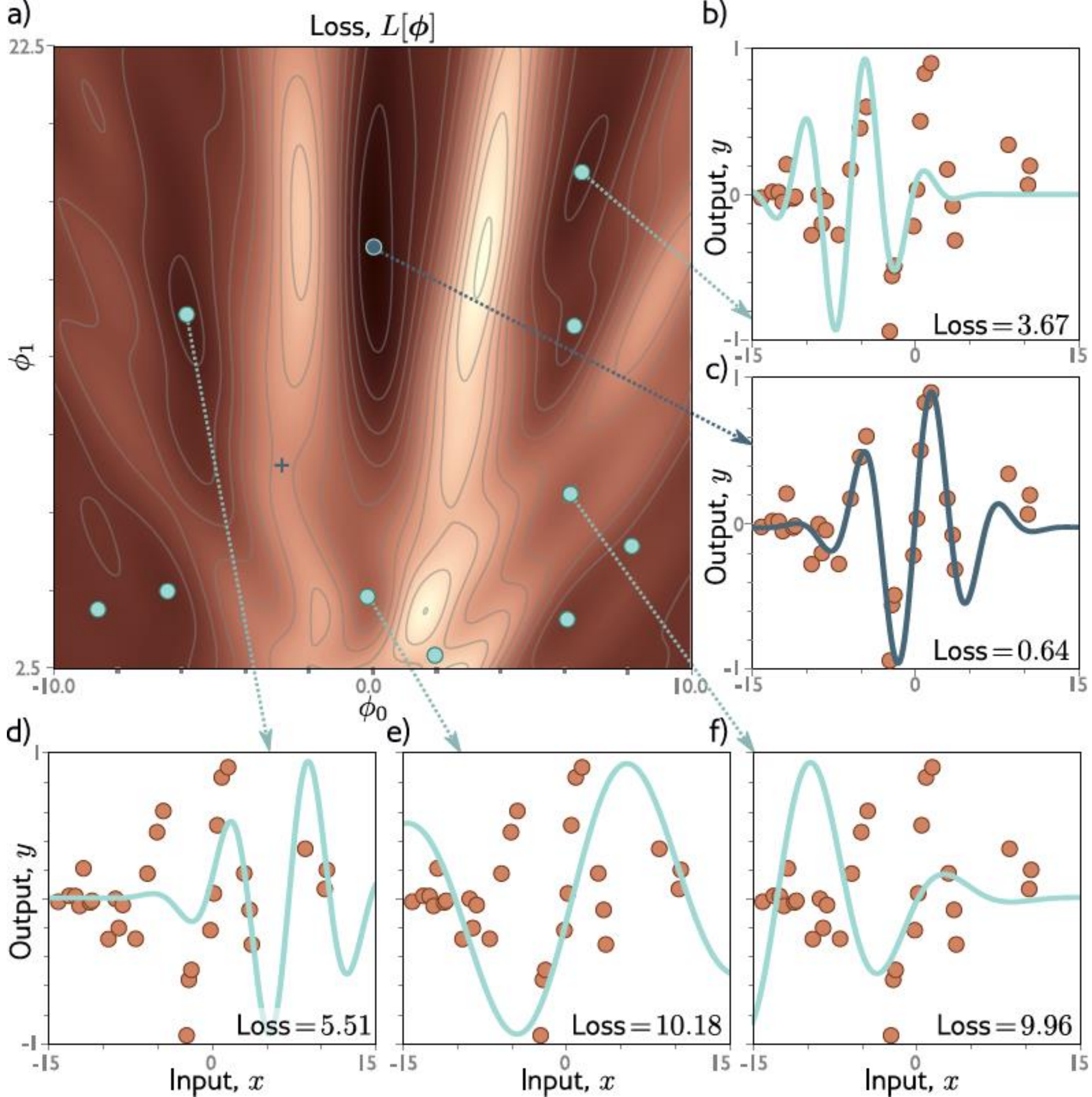
Toy Dataset and Gabor model

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



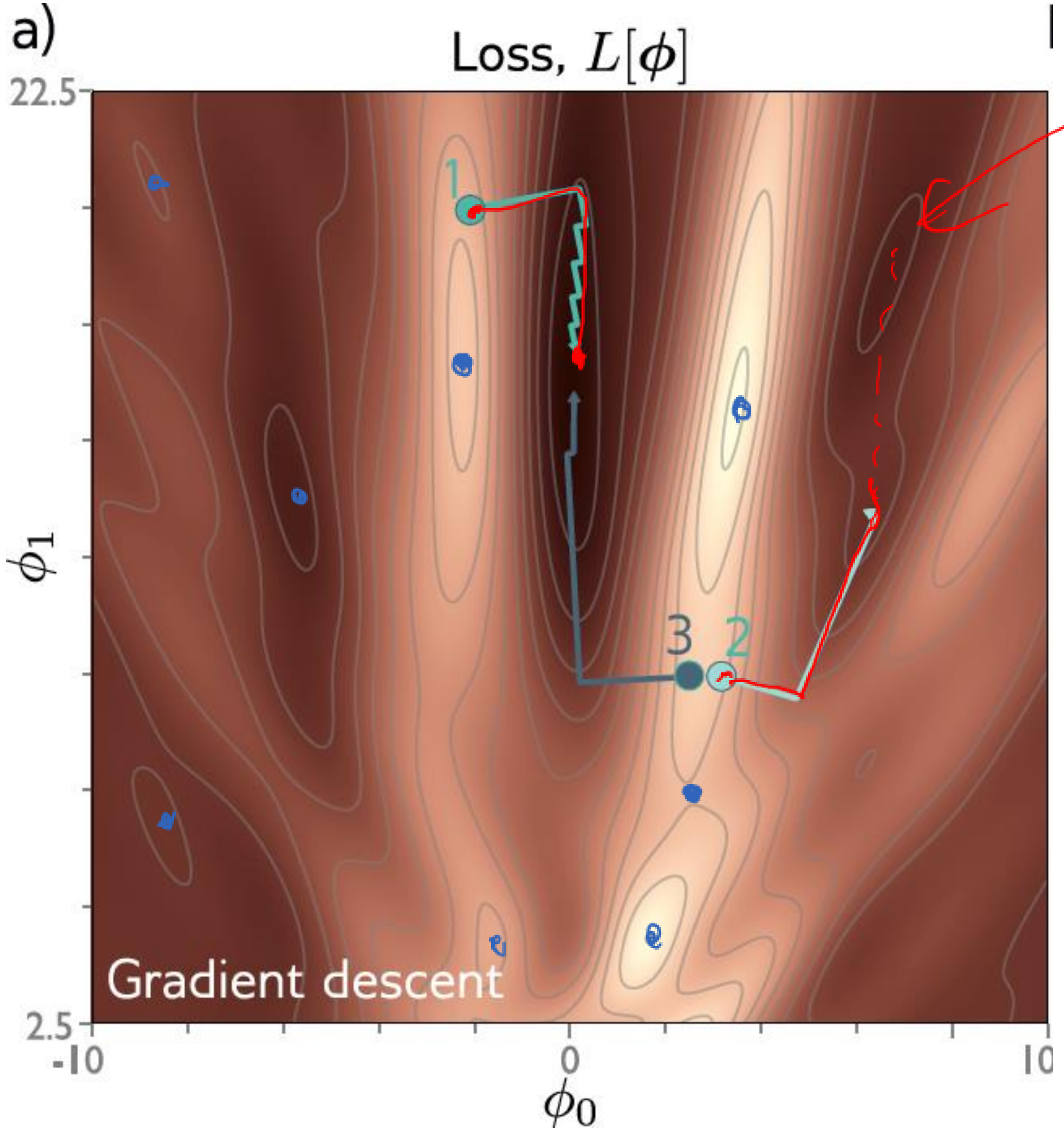


$$L[\boldsymbol{\phi}] = \sum_{i=1}^{I} \left(\mathrm{f}[x_i, \boldsymbol{\phi}] - y_i\right)^2$$



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

• = zero gradient



local minima

- 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

end point depends on start point.

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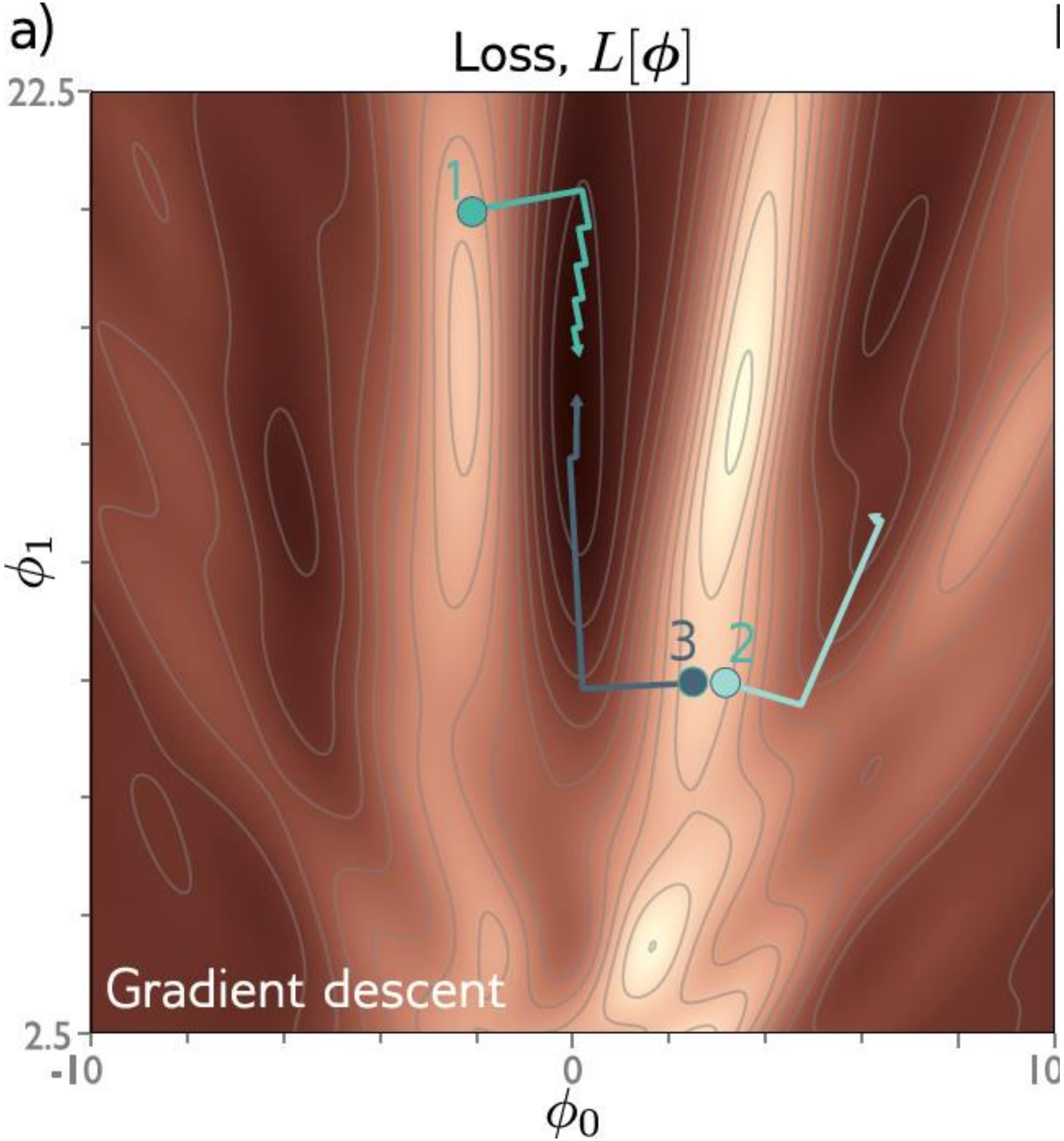


IDEA: add noise, save computation

- 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)

original data order

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]

1 st batch 2nd batch

randomize

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]
```

...

Stochastic grad

Before (full bat

After (SGD)

Fixed learning r

Stochastic gradient descent

Before (full batch descent)

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

sum over dataset

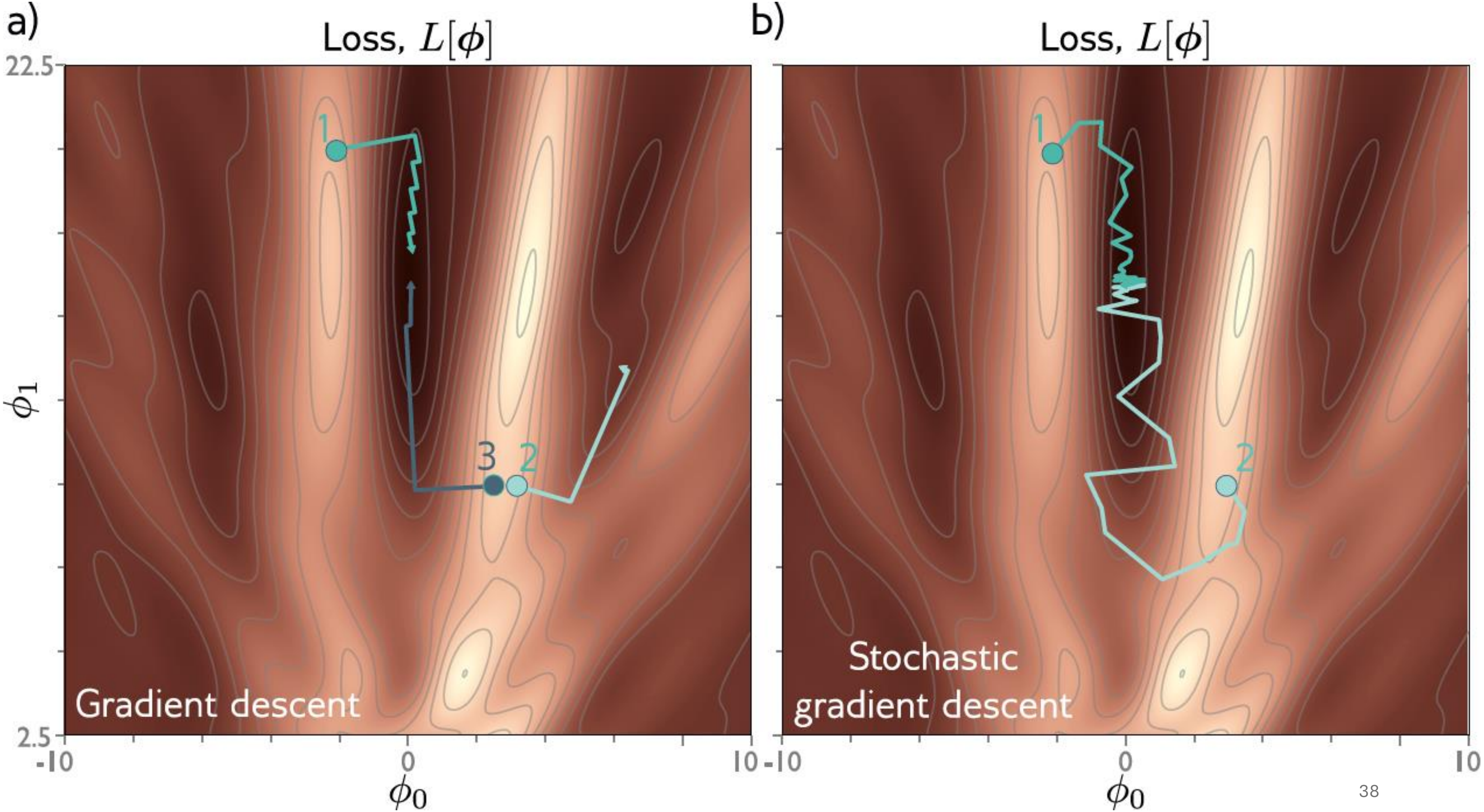
After (SGD)

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

sum over batch

Fixed learning rate α

maybe change b/w epochs


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

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

batch gradients have distribution around dataset gradient (averaging)

Same prediction/loss/gradient work, slightly more parameter update work.

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

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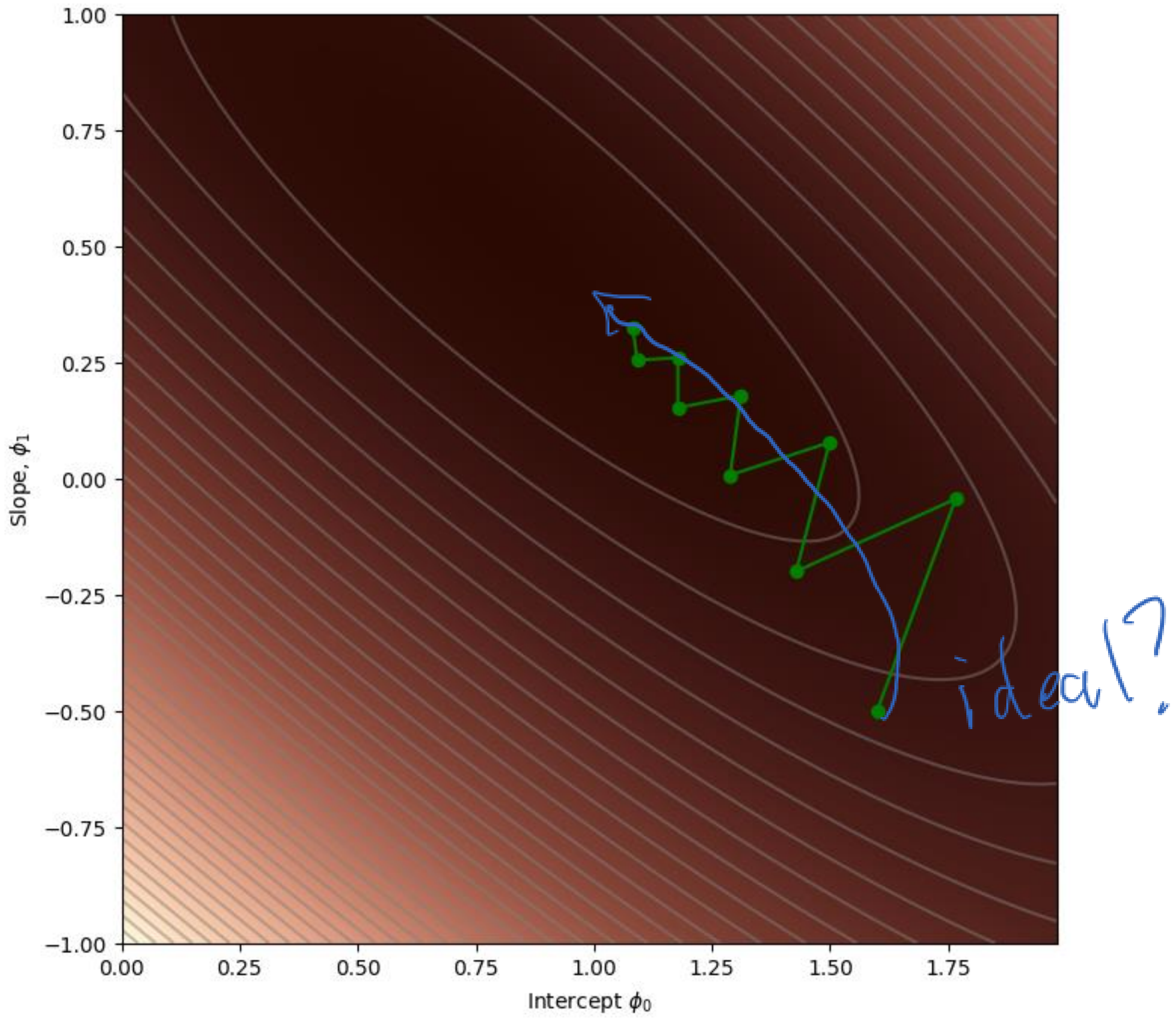
Simple Gradient Descent



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

exponentially weighted moving average

gradient

momentum

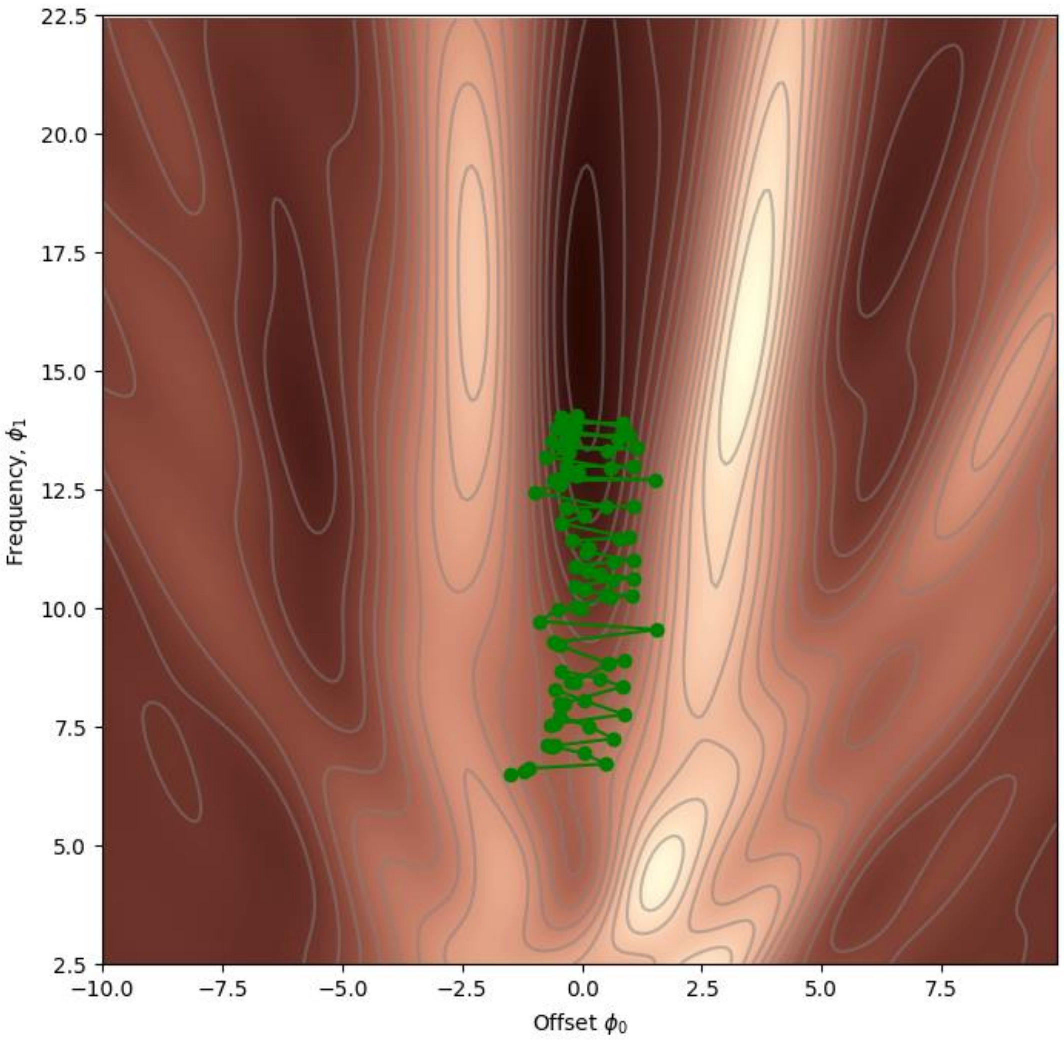
$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta) \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\phi_t]}{\partial \phi}$$

β is hyper parameter controlling momentum smoothing.

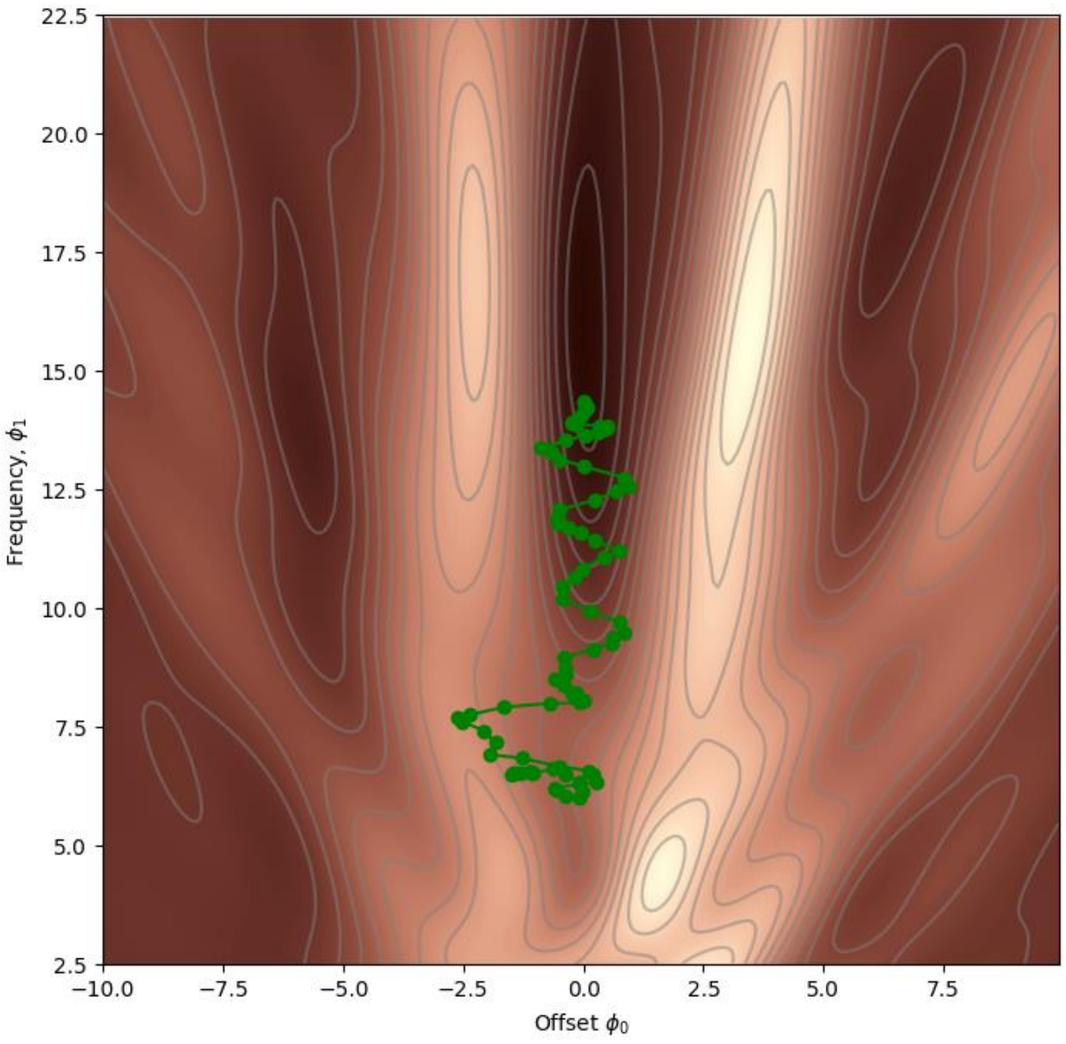
$$\phi_{t+1} \leftarrow \phi_t - \alpha \cdot \mathbf{m}_{t+1}$$

Still in batches.

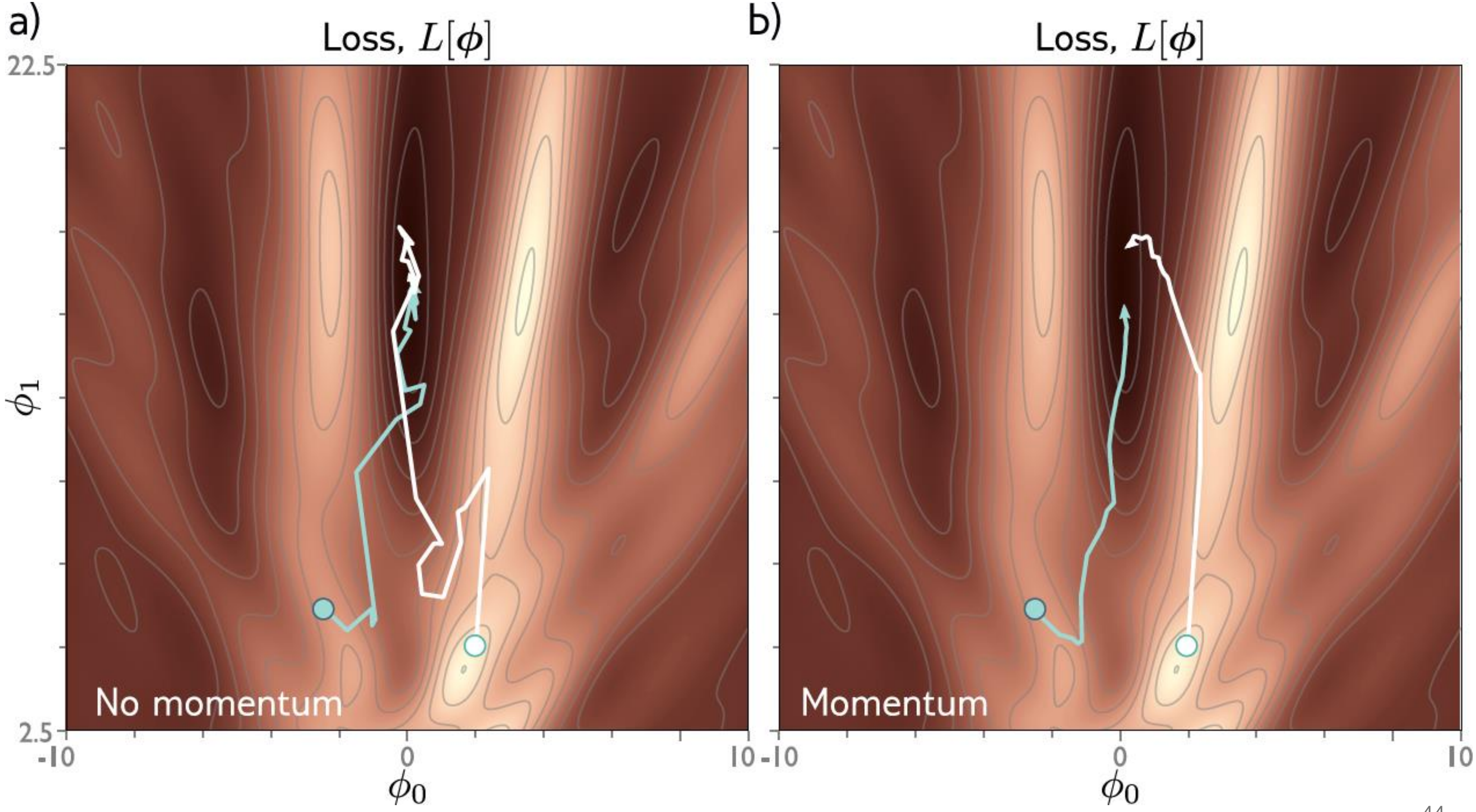
Without and With Momentum



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

"Anticipate turns instead of turning at last second"

- Momentum smooths out gradient of current location

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

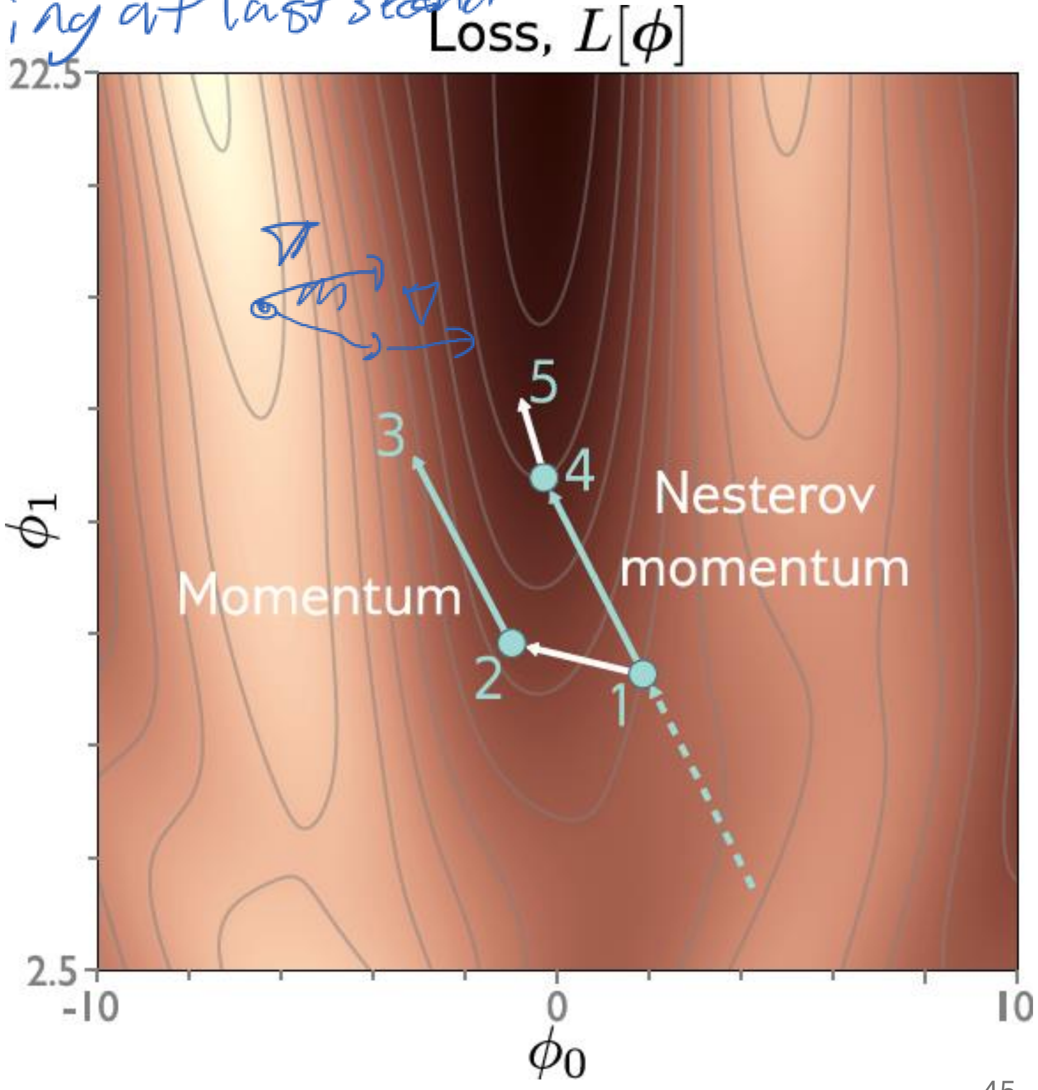
$$\boldsymbol{\phi}_{t+1} \leftarrow \boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_{t+1}$$

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

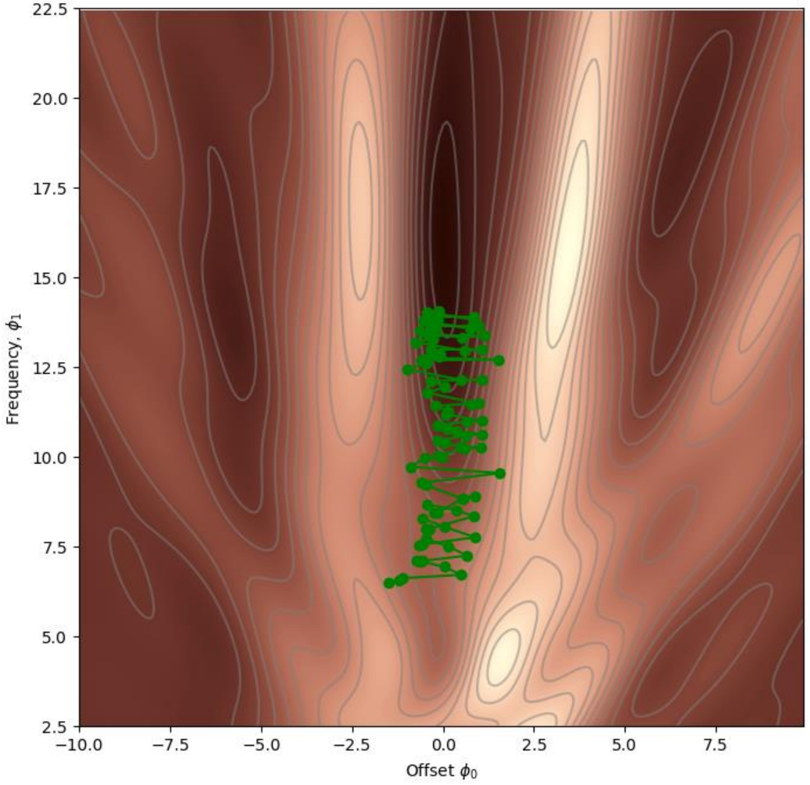
$$\mathbf{m}_{t+1} \leftarrow \beta \cdot \mathbf{m}_t + (1-\beta) \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\boldsymbol{\phi}_t - \alpha \cdot \mathbf{m}_t]}{\partial \boldsymbol{\phi}}$$

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

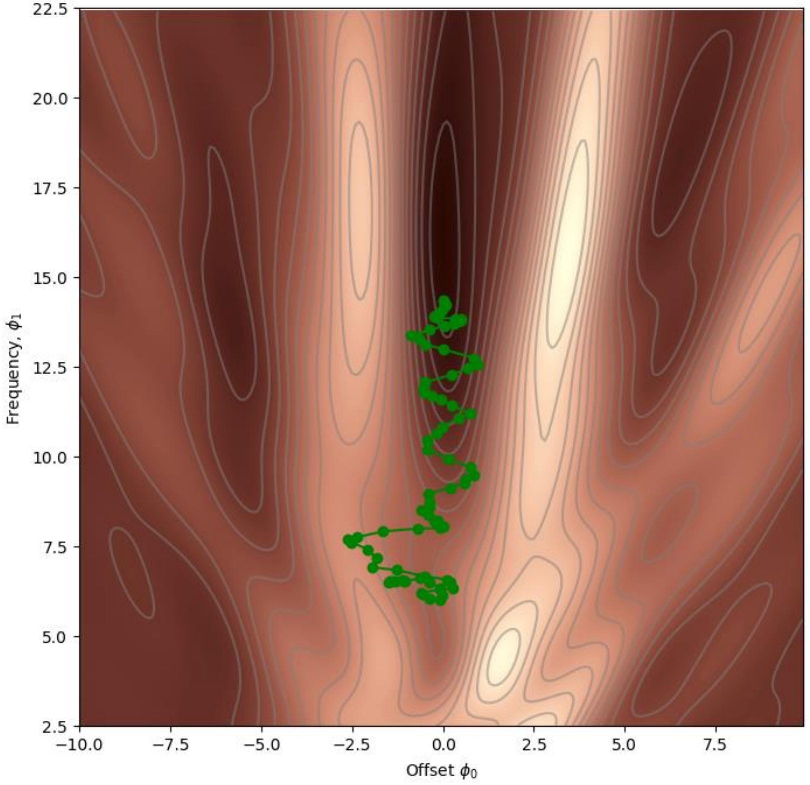
Still in batches.



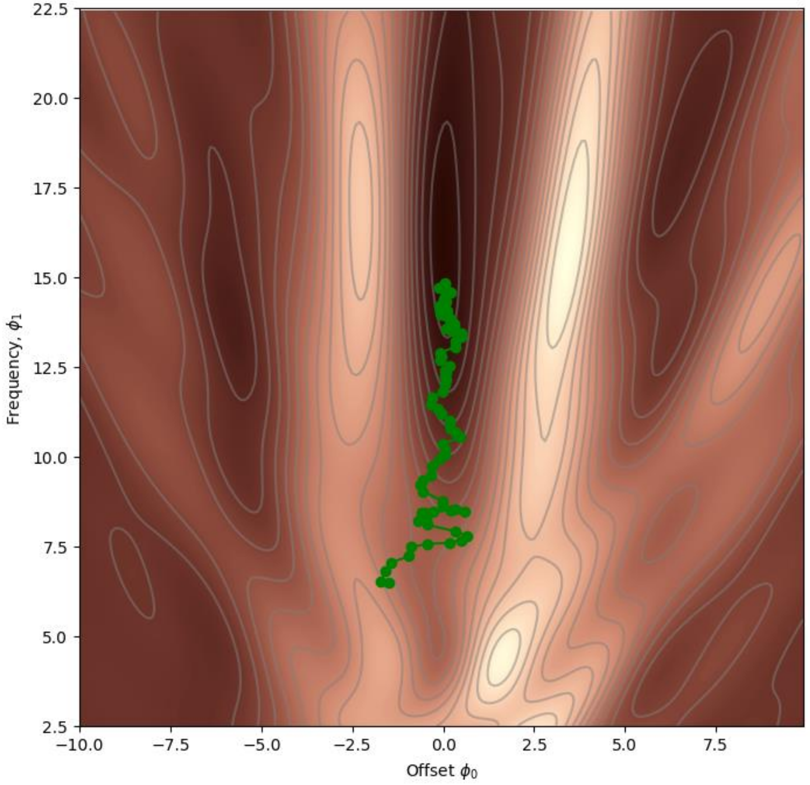
Nesterov Momentum



Without Momentum, Loss = 1.31



With Momentum, Loss = 0.96



Nesterov Momentum, Loss = 0.80

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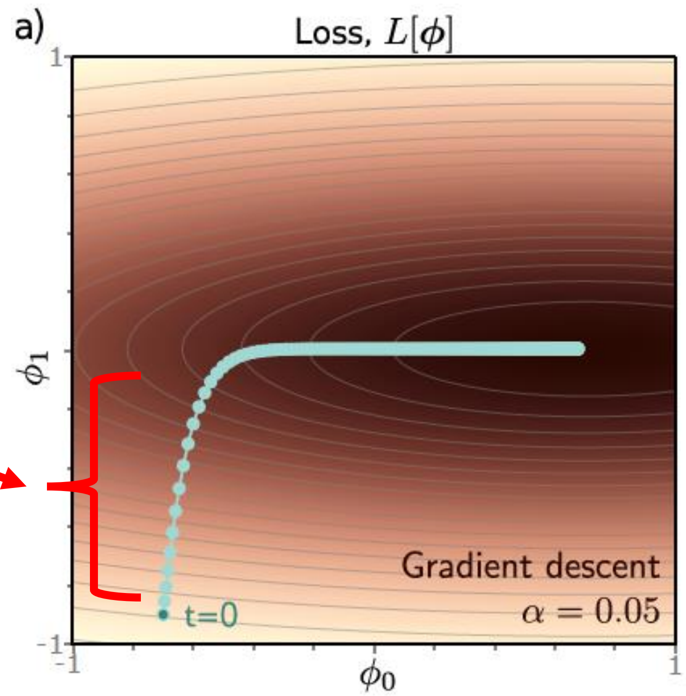
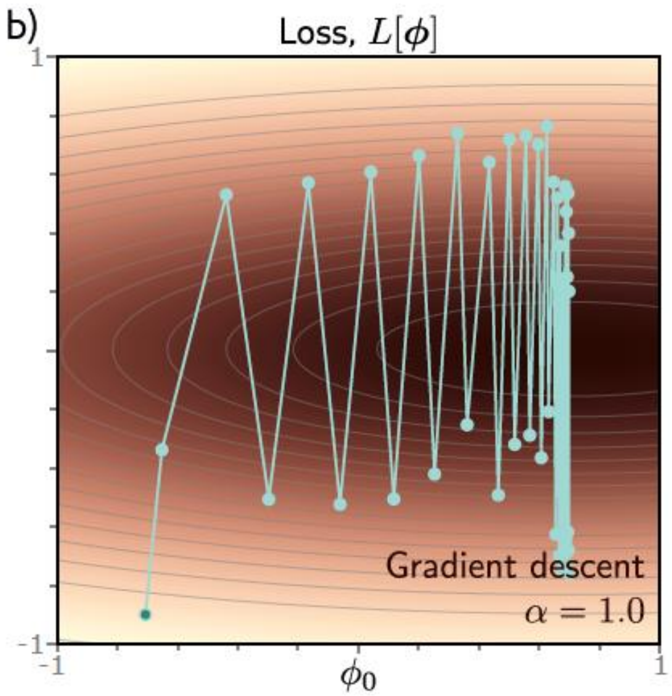
The challenge with fixed step sizes

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

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

Dividing by the magnitude, so normalized to unit vector.

Solution Part 1: Unit Vector gradients

- Measure mean and pointwise squared gradient

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

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

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

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

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

- Normalize:

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

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

Large gradient components suppress other gradient components!

Solution Part 2: Normalized gradients

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

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

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

- 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

$$\frac{m_i}{|m_i|} = 1 \text{ or } -1$$

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

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

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

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

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

- Normalize:

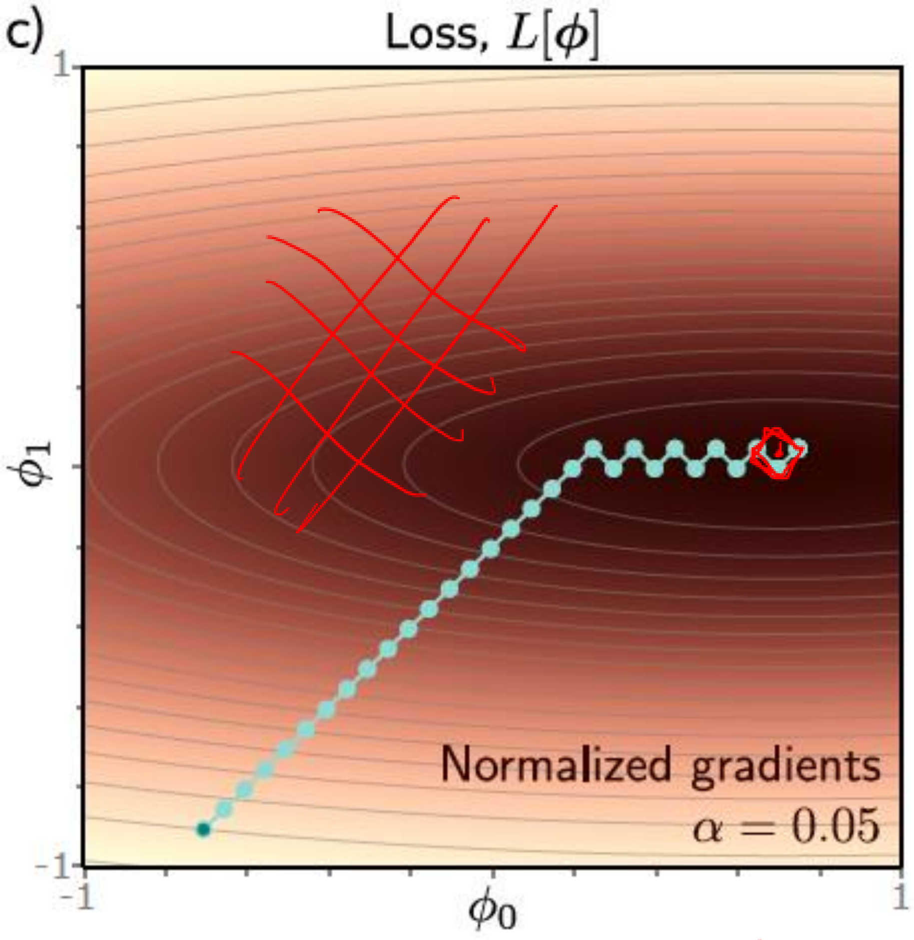
$$\phi_{t+1} \leftarrow \phi_t - \alpha \cdot \frac{\mathbf{m}_{t+1}}{\sqrt{\mathbf{v}_{t+1}} + \epsilon}$$

rare

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

Parameter changes are +1, 0, -1

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

moving on a grid in parameter space

Adaptive moment estimation (Adam)

- Compute mean and pointwise squared gradients *with momentum*

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

same momentum calc as before

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

momentum version of squared gradients

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

$$\tilde{\mathbf{m}}_{t+1} \leftarrow \frac{\mathbf{m}_{t+1}}{1-\beta^{t+1}} \qquad \mathbf{m}_{t=0} = 0$$

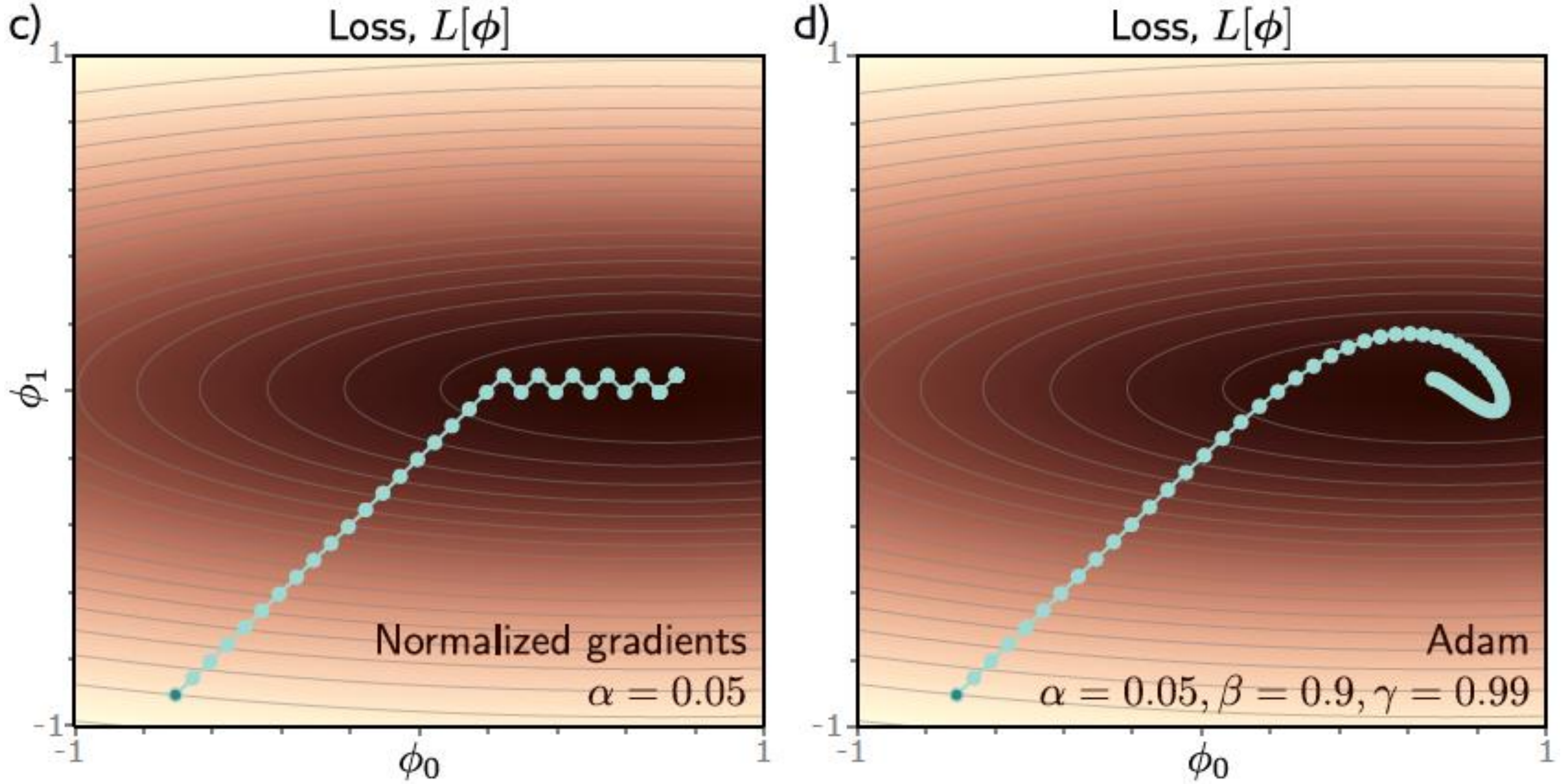
$$\tilde{\mathbf{v}}_{t+1} \leftarrow \frac{\mathbf{v}_{t+1}}{1-\gamma^{t+1}} \qquad \mathbf{v}_{t=0} = 0$$

compensate for zero init

- 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)



Other advantages of ADAM

different gradient magnitudes motivate per-parameter norm...

- 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.

counterexamples exist, but generally good enough in practice.

Additional Hyperparameters

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

  care more if SGD
- Momentum Parameters

  stick w/ PyTorch defaults.

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 imbalance between gradient components while providing some momentum