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Optimization Algorithms

Mini-batch gradient descent

Batch vs. mini-batch gradient descent

X, Y $\qquad$ $X^{\{t\}}, Y^{\{t\}}$

Vectorization allows you to efficiently compute on m examples.

$$X = [\underbrace{x^{(1)}\ x^{(2)}\ x^{(3)} \dots x^{(1000)}}_{X^{\{1\}}\ (n_x, 1000)} \mid \underbrace{x^{(1001)} \dots x^{(2000)}}_{X^{\{2\}}\ (n_x, 1000)} \mid \dots \mid \underbrace{\dots x^{(m)}}_{X^{\{5,000\}}\ (n_x, 1000)}]$$

(n_x, m)

$$Y = [\underbrace{y^{(1)}\ y^{(2)}\ y^{(3)} \dots y^{(1000)}}_{Y^{\{1\}}\ (1, 1000)} \mid \underbrace{y^{(1001)} \dots y^{(2000)}}_{Y^{\{2\}}\ (1, 1000)} \mid \dots \mid \underbrace{\dots y^{(m)}}_{Y^{\{5,000\}}\ (1, 1000)}]$$

$(1, m)$

What if $m = 5{,}000{,}000$?

5,000 mini-batches of 1,000 each

Mini-batch t: $X^{\{t\}}, Y^{\{t\}}$

$x^{(i)}$

$z^{[l]}$

$X^{\{t\}}, Y^{\{t\}}$.

Andrew Ng

Mini-batch gradient descent

1 step of gradient descent using $X^{\{t\}}, Y^{\{t\}}$. (as if $m = 1000$)

repeat {

for $t = 1, \dots, 5000$ {

Forward prop on $X^{\{t\}}$.

$$Z^{[1]} = W^{[1]} X^{\{t\}} + b^{[1]}$$

$$A^{[1]} = g^{[1]}(Z^{[1]})$$

$$\vdots$$

$$A^{[L]} = g^{[L]}(Z^{[L]})$$

Vectorized implementation (1000 examples)

from $X^{\{t\}}, Y^{\{t\}}$.

Compute cost $J^{\{t\}} = \frac{1}{1000} \sum_{i=1}^{l} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2 \cdot 1000} \sum_{l} \|W^{[l]}\|_F^2$.

Backprop to compute gradients wrt $J^{\{t\}}$ (using $(X^{\{t\}}, Y^{\{t\}})$)

$W^{[l]} := W^{[l]} - \alpha dW^{[l]}$, $b^{[l]} := b^{[l]} - \alpha db^{[l]}$

}

}

"1 epoch"

pass through training set.

X, Y

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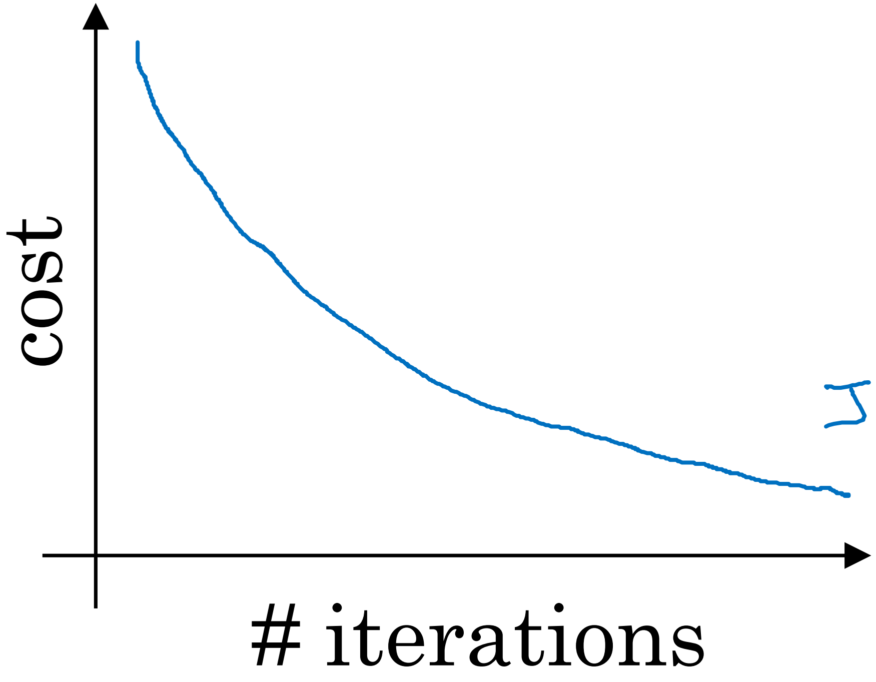
Optimization Algorithms

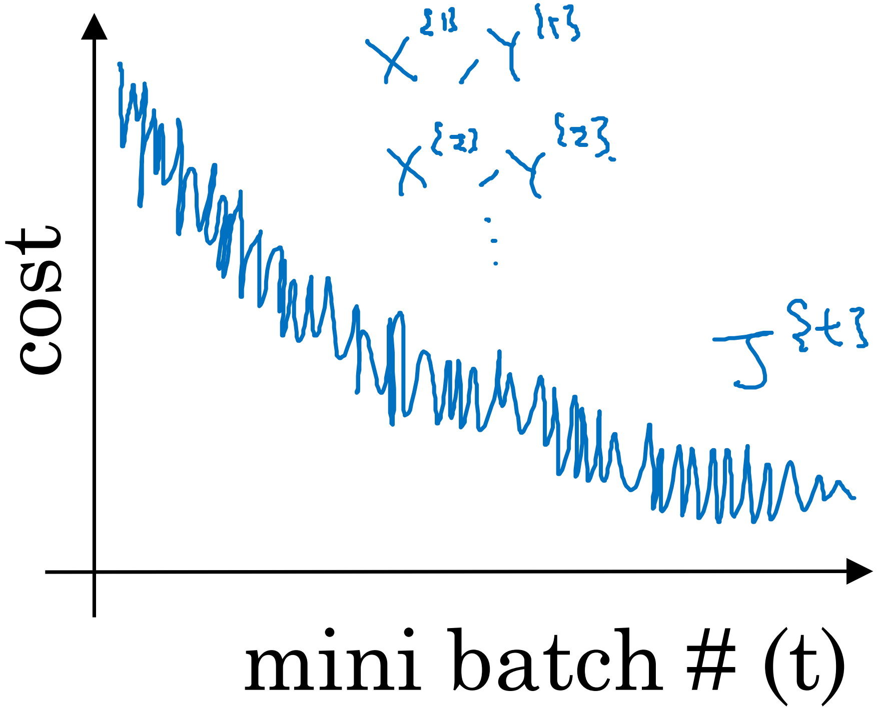
Understanding mini-batch gradient descent

Training with mini batch gradient descent

Batch gradient descent



Mini-batch gradient descent



Plot $J^{\{t\}}$ computed using $\underline{X^{\{t\}}, Y^{\{t\}}}$

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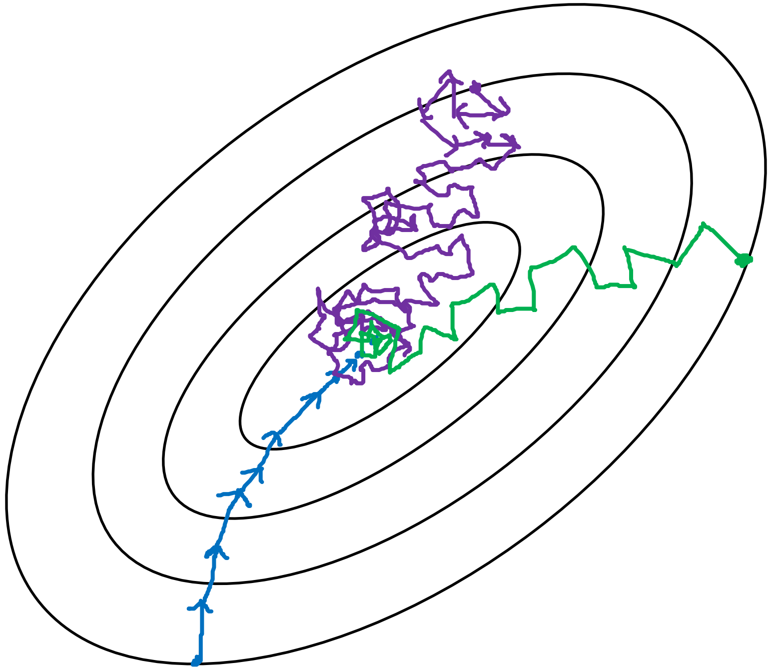
Choosing your mini-batch size

→ If mini-batch size = m : Batch gradient descent. $(X^{\{1\}}, Y^{\{1\}}) = (X, Y)$.

→ If mini-batch size = 1 : Stochastic gradient descent. Every example is it own mini-batch.
$(X^{\{1\}}, Y^{\{1\}}) = (x^{(1)}, y^{(1)}) \dots (x^{(2)}, y^{(2)})$ mini-batch.

In practice: Somewhere in-between $\underline{1}$ and $\underline{m}$



Stochastic gradient descent

$\Downarrow$

Lose speedup from vectorization

In-between (mini-batch size not too big/small)

$\Downarrow$

Fastest learning.

- Vectorization. (~1000)
- Make progress without processing entire training set.

Batch gradient descent (mini-batch size = m)

$\Downarrow$

Too long per iteration

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Choosing your mini-batch size

If small train set: Use batch gradient descent.
$(m \leq 2000)$

Typical mini-batch sizes:

$\rightarrow \underbrace{\underset{2^6}{64}, \underset{2^7}{128}, \underset{2^8}{256}, \underset{2^9}{512}} \qquad \frac{1024}{2^{10}}$

Make sure mini-batch fit in CPU/GPU memory.
$X^{\{t\}}, Y^{\{t\}}$

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Optimization Algorithms

Exponentially weighted averages

Temperature in London

$\theta_1 = 40°F$ 4°C ←

$\theta_2 = 49°F$ 9°C

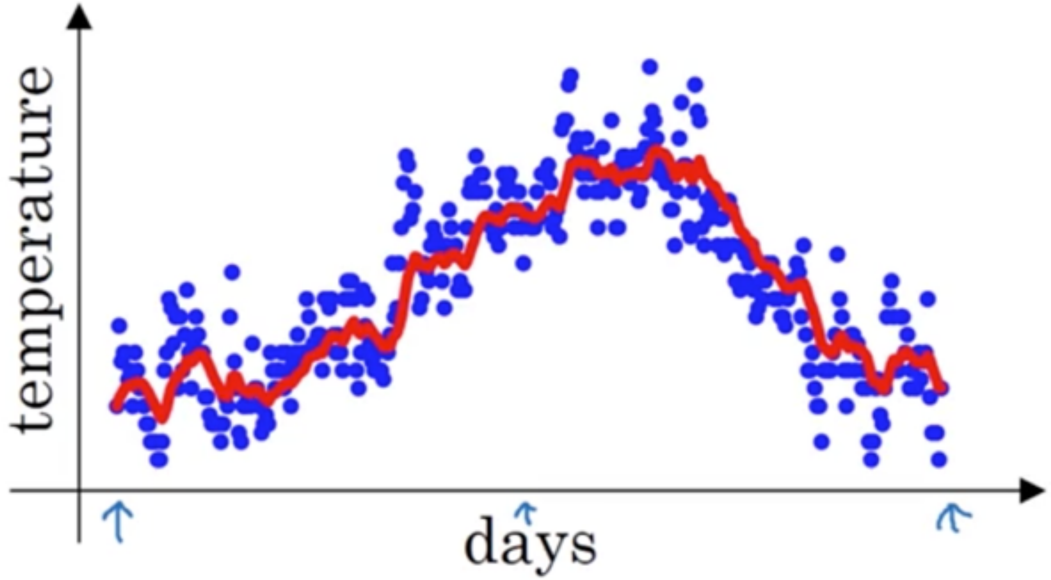
$\theta_3 = 45°F$ ⋮

⋮

$\theta_{180} = 60°F$ 15°C

$\theta_{181} = 56°F$ ⋮

⋮



$V_0 = 0$

$V_1 = 0.9\,V_0 + 0.1\,\theta_1$

$V_2 = 0.9\,V_1 + 0.1\,\theta_2$

$V_3 = 0.9\,V_2 + 0.1\,\theta_3$

⋮

$V_t = 0.9\,V_{t-1} + 0.1\,\theta_t$

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Exponentially weighted averages

moving

$$V_t = \beta V_{t-1} + (1-\beta)\theta_t \leftarrow$$

$\beta = 0.9$: ≈ 10 days' temperature.

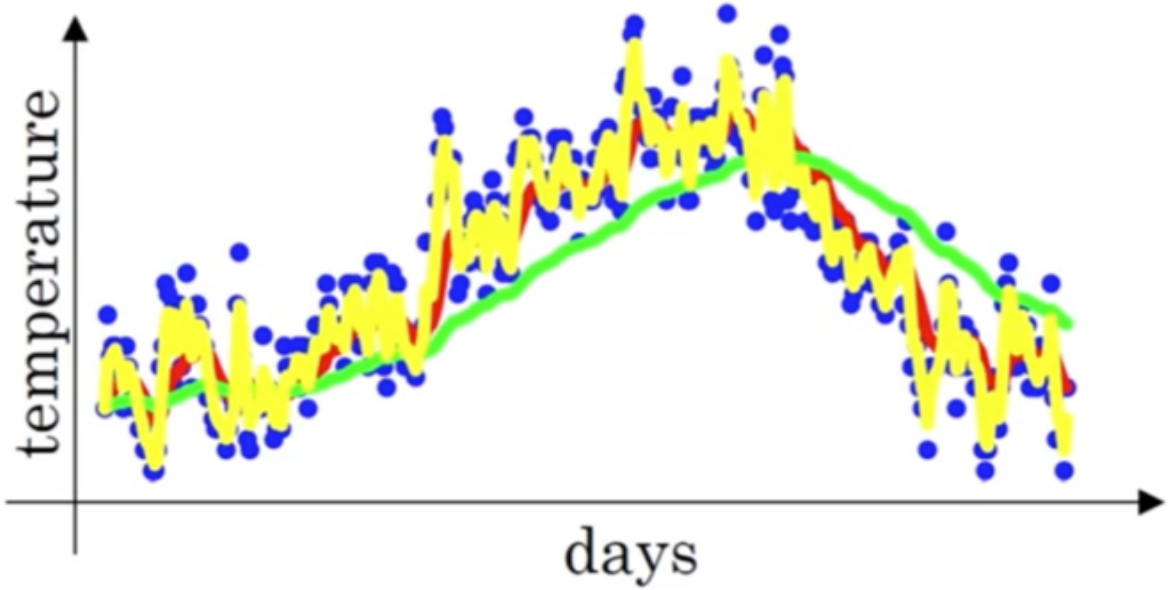
$\beta = 0.98$: ≈ 50 days

$\beta = 0.5$: ≈ 2 days

V_t as approximately average over

$\rightarrow \approx \frac{1}{1-\beta}$ days' temperature.

$$\frac{1}{1-0.98} = 50$$



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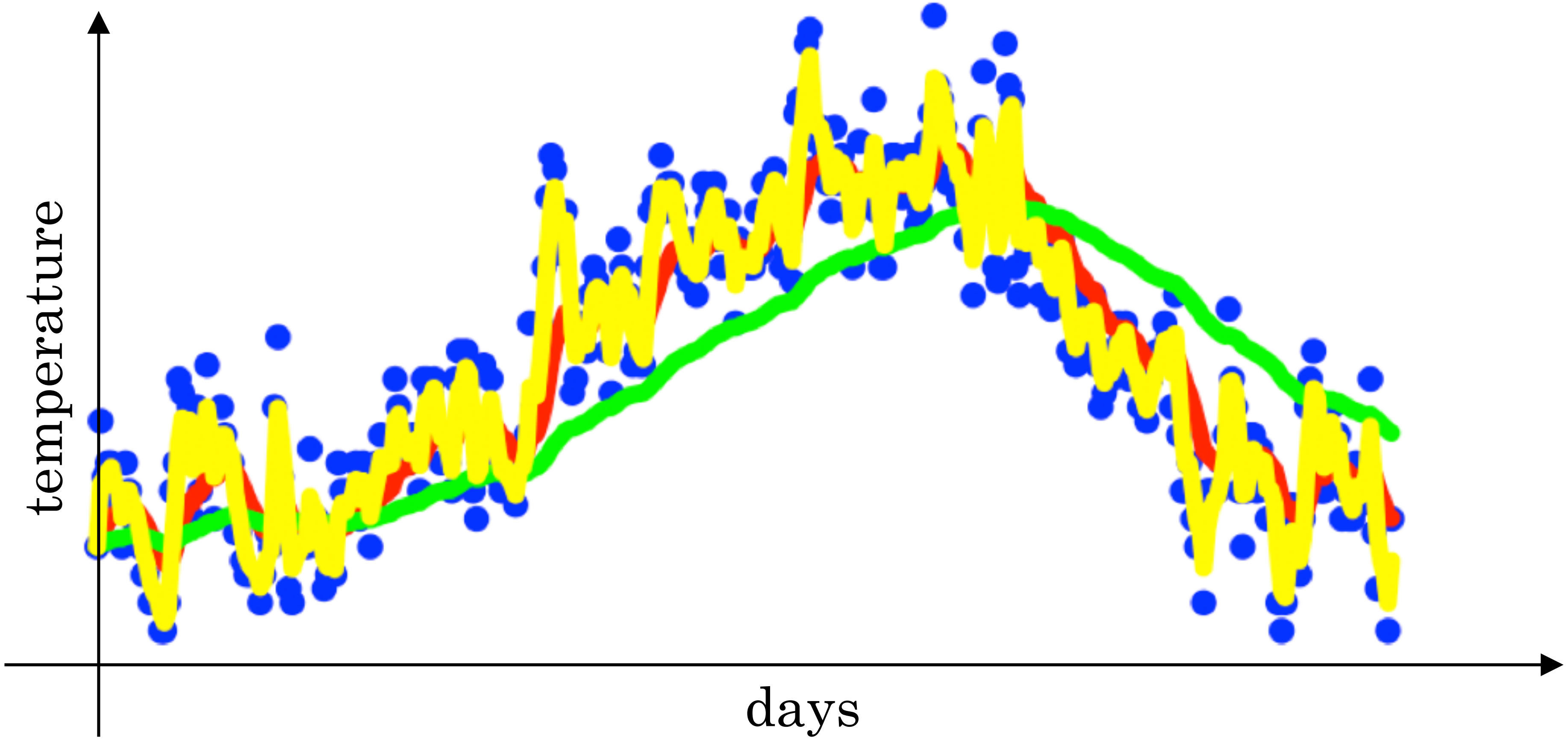
Optimization Algorithms

Understanding exponentially weighted averages

Exponentially weighted averages

$$\boxed{v_t = \beta v_{t-1} + (1-\beta)\theta_t}$$

$\beta = 0.9$ 0.98 0.5



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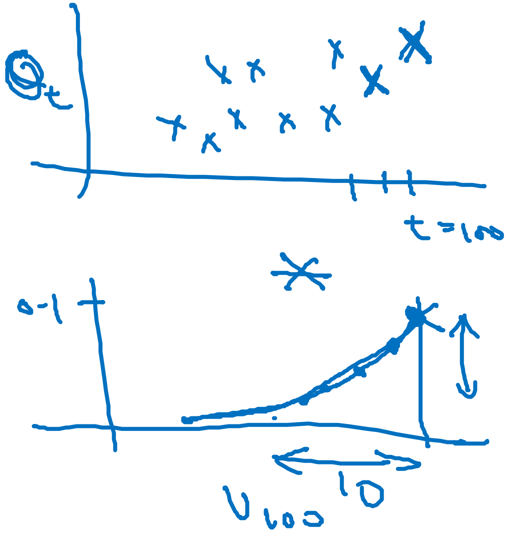
Exponentially weighted averages

$$v_t = \beta v_{t-1} + (1-\beta)\theta_t$$



$$\approx \frac{1}{1-\beta}$$

$$\varepsilon = 1-\beta$$

$$v_{100} = 0.9v_{99} + 0.1\theta_{100}$$

$$\boxed{v_{99} = 0.9v_{98} + 0.1\theta_{99}}$$

$$\boxed{v_{98} = 0.9v_{97} + 0.1\theta_{98}}$$

...

$$0.1\,\theta_{98} + 0.9\,v_{97}$$

$$v_{100} = 0.1\,\theta_{100} + 0.9\,\cancel{v_{99}}\left(0.1\,\theta_{99} + 0.9\,\cancel{v_{98}}\right)$$

$$= 0.1\,\theta_{100} + 0.1 \times 0.9 \cdot \theta_{99} + 0.1\,(0.9)^2\,\theta_{98} + 0.1\,(0.9)^3\,\theta_{97} + 0.1\,(0.9)^4\,\theta_{96} + \dots$$

$$0.9^{10} \approx 0.35 \approx \frac{1}{e}$$

$$\underbrace{(1-\varepsilon)}_{0.9}{}^{1/\varepsilon} = \frac{1}{e}$$

$$0.98 \,?$$

$$\varepsilon = 0.02 \rightarrow 0.98^{50} \approx \frac{1}{e}$$

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Implementing exponentially weighted averages

$$v_0 = 0$$
$$v_1 = \beta v_0 + (1-\beta)\,\theta_1$$
$$v_2 = \beta v_1 + (1-\beta)\,\theta_2$$
$$v_3 = \beta v_2 + (1-\beta)\,\theta_3$$
$$\ldots$$

$V_\theta := 0$

$V_\theta := \beta v + (1-\beta)\,\theta_1$

$V_\theta := \beta v + (1-\beta)\,\theta_2$

$\vdots$

$\rightarrow V_\theta = 0$

Repeat {

Get next θ_t

$V_\theta := \beta V_\theta + (1-\beta)\,\theta_t \leftarrow$

}

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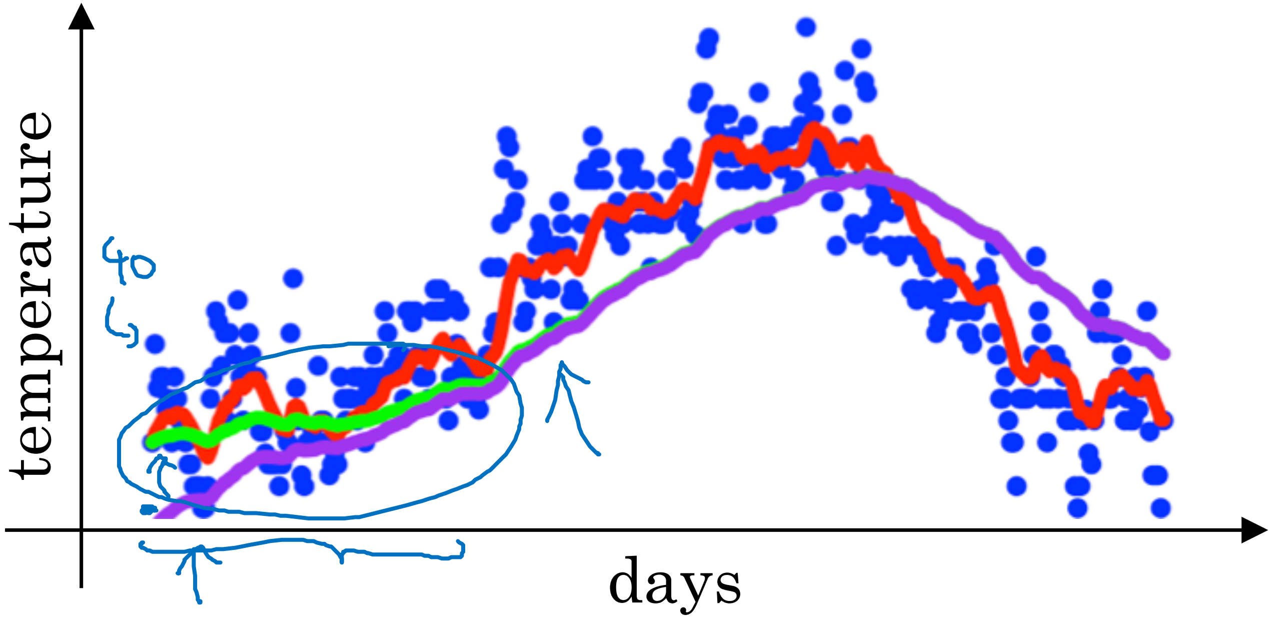
Optimization Algorithms

Bias correction in exponentially weighted average

Bias correction



$\beta = 0.98$

$\rightarrow v_t = \beta v_{t-1} + (1-\beta)\theta_t$

$V_0 = 0$

$V_1 = \cancel{0.98 V_0 +} \; 0.02\,\theta_1$

$V_2 = 0.98\,V_1 + 0.02\,\theta_2$

$= 0.98 \times 0.02 \times \theta_1 + 0.02\,\theta_2$

$= 0.0196\,\theta_1 + 0.02\,\theta_2$

$\frac{V_t}{1-\beta^t}$

$t=2: \quad 1-\beta^t = 1-(0.98)^2 = 0.0396$

$\frac{V_2}{0.0396} = \frac{0.0196\,\theta_1 + 0.02\,\theta_2}{0.0396}$

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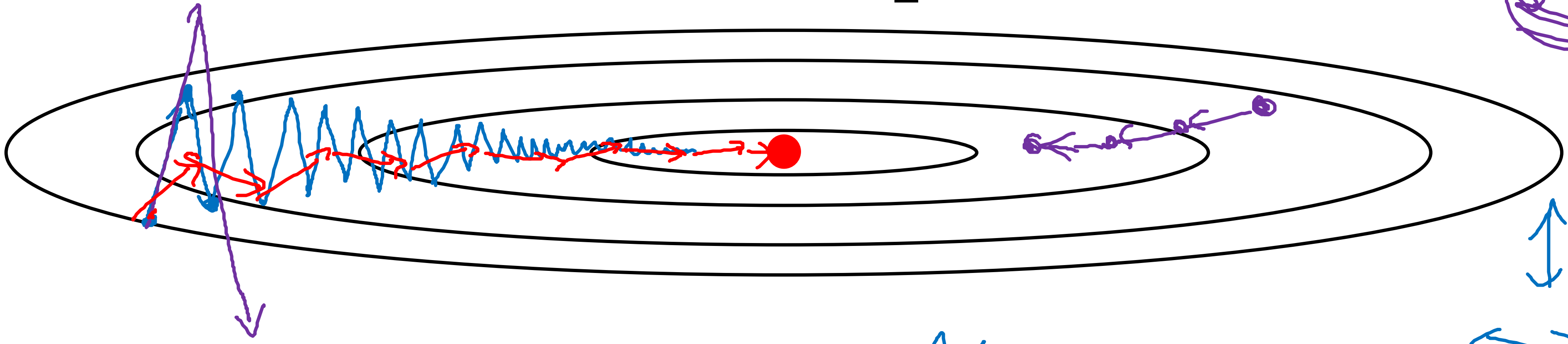
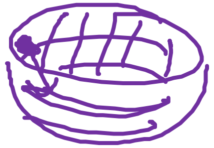
Optimization Algorithms

Gradient descent with momentum

Gradient descent example





slower learning

faster learning

Momentum:

On iteration t:

Compute dW, db on current mini-batch.

$$V_{dw} = \beta V_{dw} + (1-\beta)\, dW$$

"$V_\theta = \beta V_\theta + (1-\beta)\, \theta_t$"

$$V_{db} = \beta V_{db} + (1-\beta)\, db$$

friction — velocity — acceleration

$$W := W - \alpha V_{dw}, \quad b := b - \alpha V_{db}$$

Implementation details

$V_{dw} = 0$, $V_{db} = 0$

On iteration t:

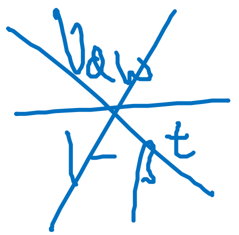
Compute dW, db on the current mini-batch

$$v_{dW} = \beta v_{dW} + \cancel{(1-\beta)}dW$$

$$v_{db} = \beta v_{db} + \cancel{(1-\beta)}db$$

$$W = W - \alpha v_{dW}, \quad b = b - \alpha v_{db}$$

$V_{dw} = \beta V_{dw} + dW$



Hyperparameters: α, β

$\beta = 0.9$

average over last ≈ 10 gradients

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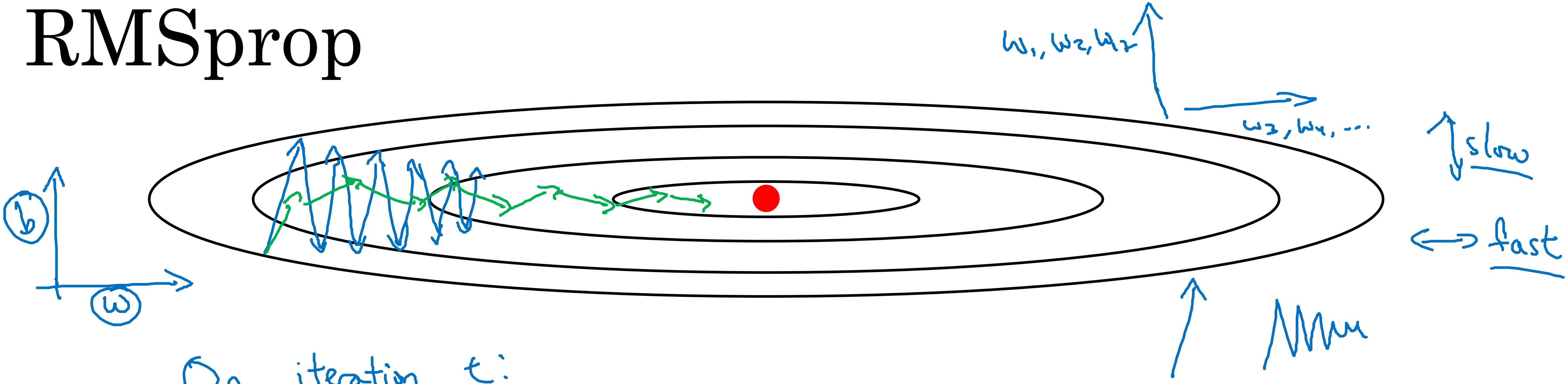
Optimization Algorithms

RMSprop

RMSprop



On iteration t:

Compute dW, db on current mini-batch

element-wise

$S_{dW} = \beta_2 S_{dW} + (1-\beta_2)\, dW^2$ ← small

→ $S_{db} = \beta_2 S_{db} + (1-\beta_2)\, db^2$ ← large

$W := W - \alpha \dfrac{dW}{\sqrt{S_{dW}+\varepsilon}}$ ← $\qquad$ $b := b - \alpha \dfrac{db}{\sqrt{S_{db}+\varepsilon}}$ ←

$\varepsilon = 10^{-8}$

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Optimization Algorithms

Adam optimization algorithm

Adam optimization algorithm

$V_{dw}=0,\ S_{dw}=0.\quad V_{db}=0,\ S_{db}=0$

On iteration t:

Compute dW, db using current mini-batch

$V_{dw}=\beta_1 V_{dw}+(1-\beta_1)dW,\quad V_{db}=\beta_1 V_{db}+(1-\beta_1)db \leftarrow$ "momentum" β_1

$S_{dw}=\beta_2 S_{dw}+(1-\beta_2)dW^2,\quad S_{db}=\beta_2 S_{db}+(1-\beta_2)db \leftarrow$ "RMSprop" β_2

yhat = np.array([.9, 0.2, 0.1, .4, .9])

$V_{dw}^{corrected}=V_{dw}/(1-\beta_1^t),\quad V_{db}^{corrected}=V_{db}/(1-\beta_1^t)$

$S_{dw}^{corrected}=S_{dw}/(1-\beta_2^t),\quad S_{db}^{corrected}=S_{db}/(1-\beta_2^t)$

$$W:=W-\alpha\frac{V_{dw}^{corrected}}{\sqrt{S_{dw}^{corrected}}+\varepsilon}\qquad b:=b-\alpha\frac{V_{db}^{corrected}}{\sqrt{S_{db}^{corrected}}+\varepsilon}$$

Hyperparameters choice:

→ α : needs to be tune

→ β_1 : 0.9 → (dw)

→ β_2 : 0.999 → (dw^2)

→ ε : 10^{-8}

Adam : Adaptive moment estimation

Adam Coates

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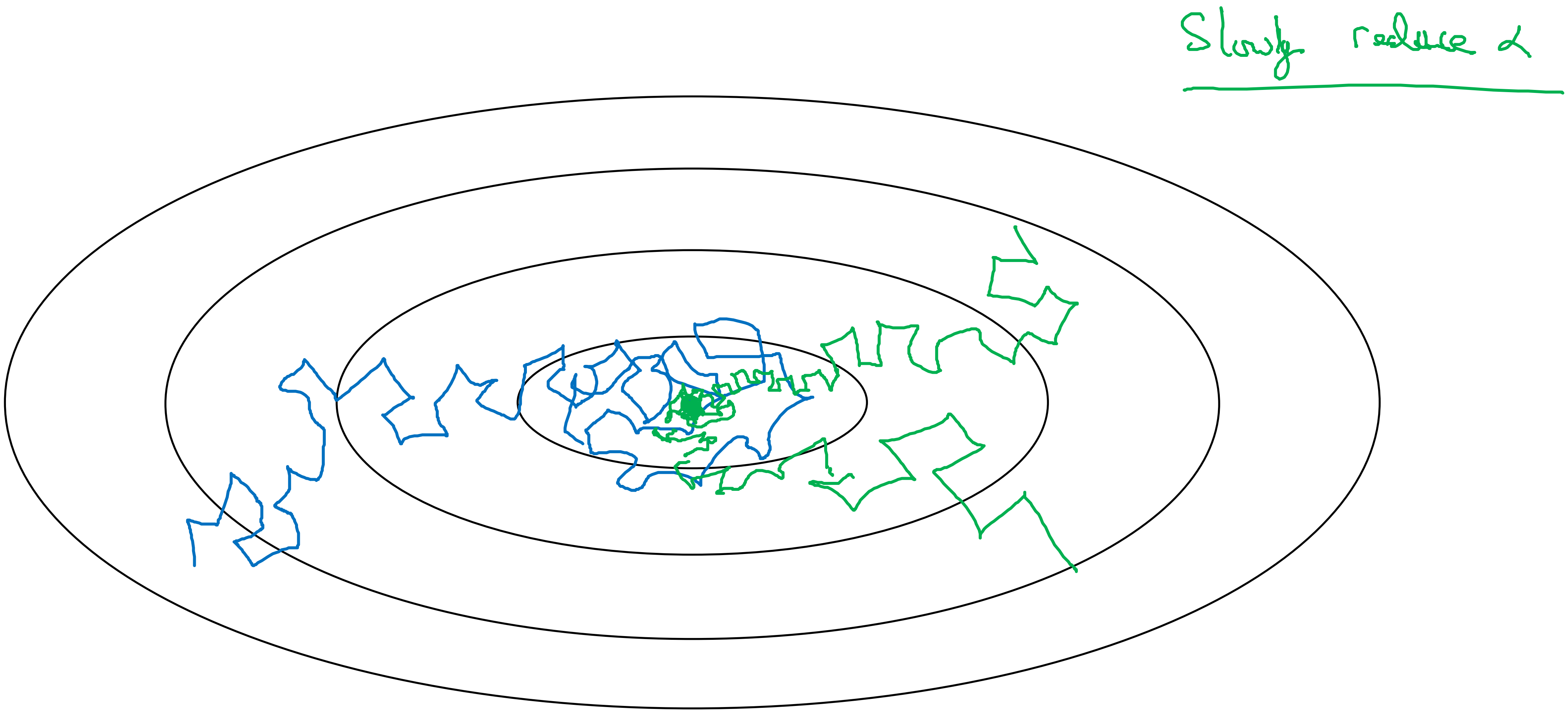
Optimization Algorithms

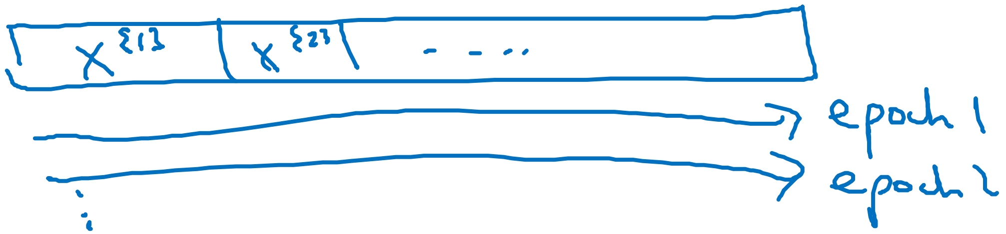
Learning rate decay

Learning rate decay



Learning rate decay

1 epoch = 1 pass through data.

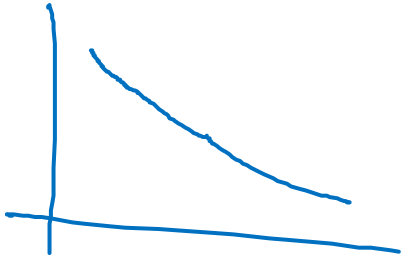


$$\alpha = \frac{1}{1 + \text{decay-rate} * \text{epoch-num}} \alpha_0$$

Epoch	α
1	0.1
2	0.67
3	0.5
4	0.4
$\vdots$	$\vdots$

$\alpha_0 = 0.2$

decay-rate $= 1$



Other learning rate decay methods

formula

$$\alpha = 0.95^{\text{epoch-num}} \cdot \alpha_0$$ — exponentially decay.

$$\alpha = \frac{k}{\sqrt{\text{epoch-num}}} \cdot \alpha_0 \quad \text{or} \quad \frac{k}{\sqrt{t}} \cdot \alpha_0$$

discrete staircase

Manual decay.

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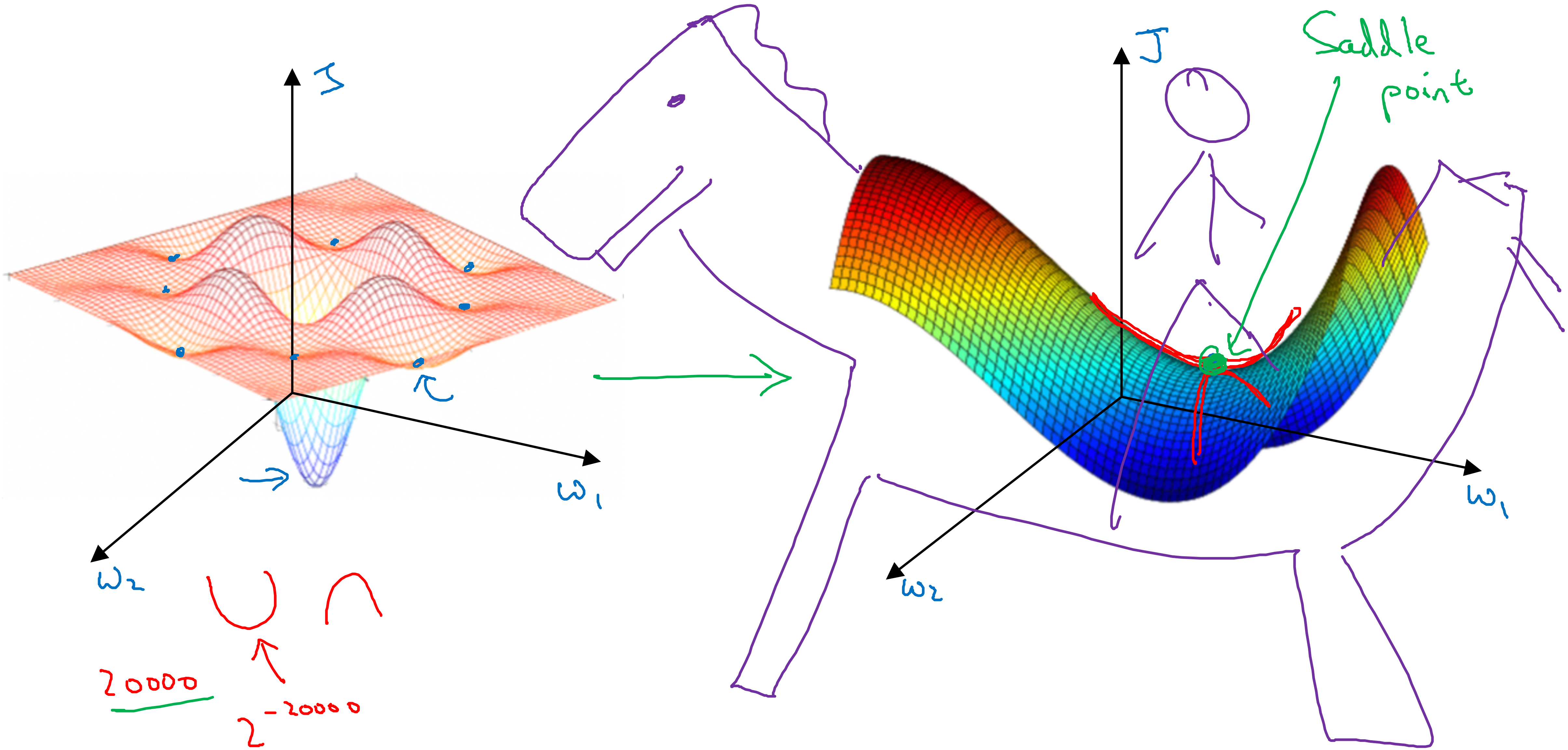
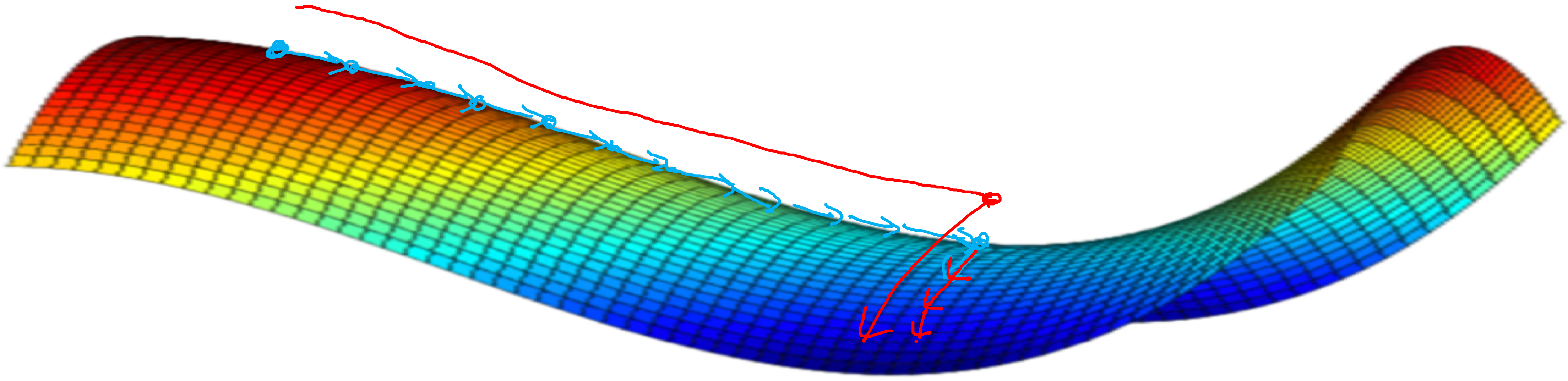
Optimization Algorithms

The problem of local optima

Local optima in neural networks



Problem of plateaus



- Unlikely to get stuck in a bad local optima
- Plateaus can make learning slow