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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 $m = 1000$)

X, Y

repeat {

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

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)

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

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

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.

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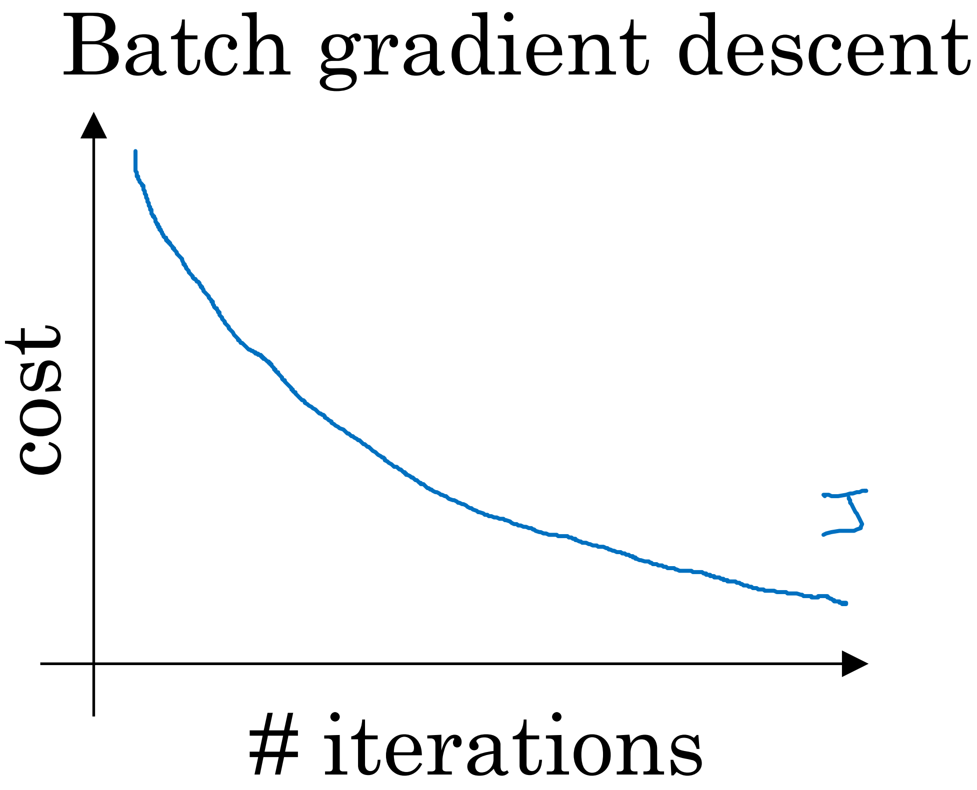
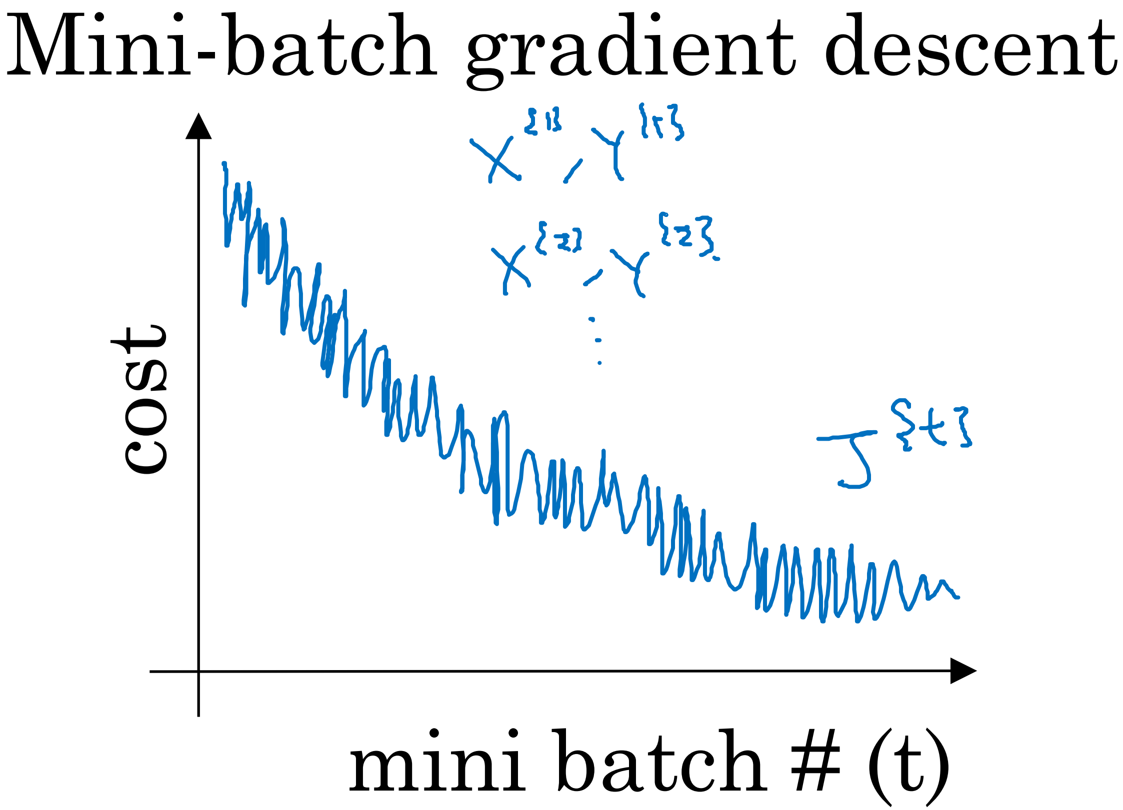
Optimization Algorithms

Understanding mini-batch gradient descent

Training with mini batch gradient descent





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

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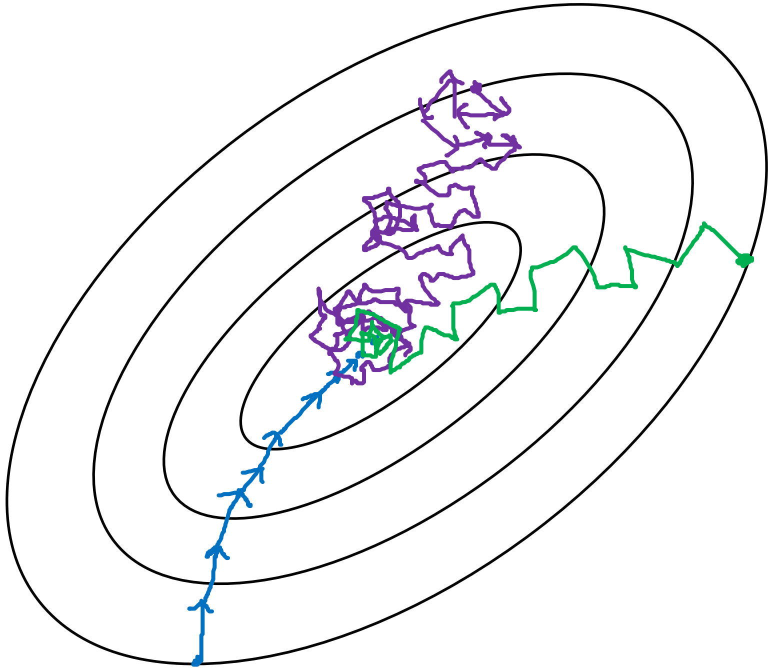
Choosing your mini-batch size

→ 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
$(X^{\{1\}}, Y^{\{1\}}) = (x^{(1)}, y^{(1)})$ … $(x^{(2)}, y^{(2)})$ mini-batch.

In practice: Somewhere in-between 1 and m



Stochastic gradient descent

⇓

Lose speedup from vectorization

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

⇓

Fastest learning.

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

Batch gradient descent (mini-batch size = m)

⇓

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:

→ 64, 128, 256, 512   1024

$\underbrace{2^6 \quad 2^7 \quad 2^8 \quad 2^9} \qquad \overline{2^{10}}$

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

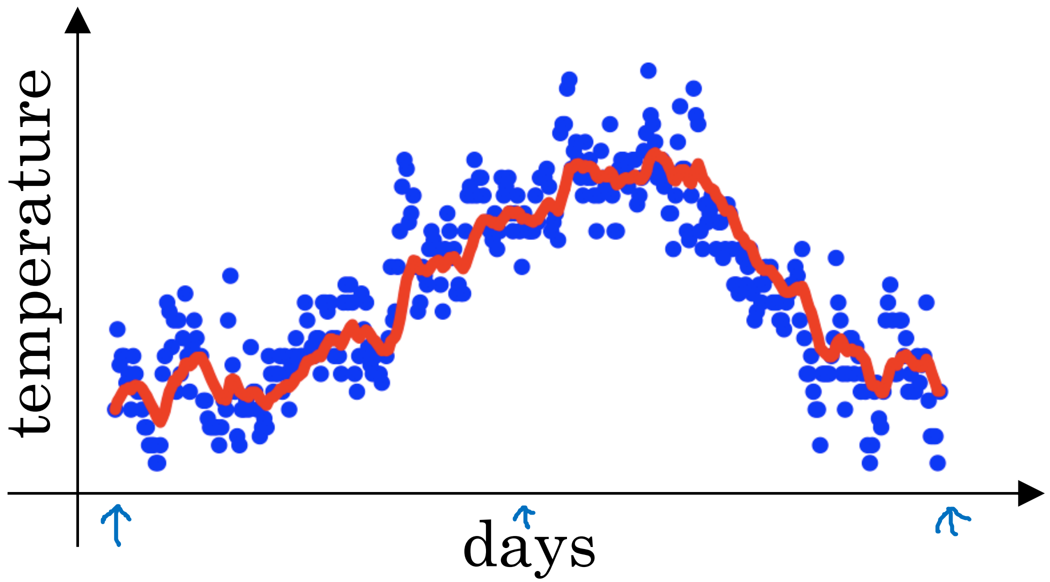
$\theta_3 = 45°F$ ⋮

⋮

$\theta_{180} = 60°F$ 15°C

$\theta_{181} = 56°F$ ⋮

⋮



$V_0 = 0$

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

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

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

⋮

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

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Exponentially weighted (moving) averages

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

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

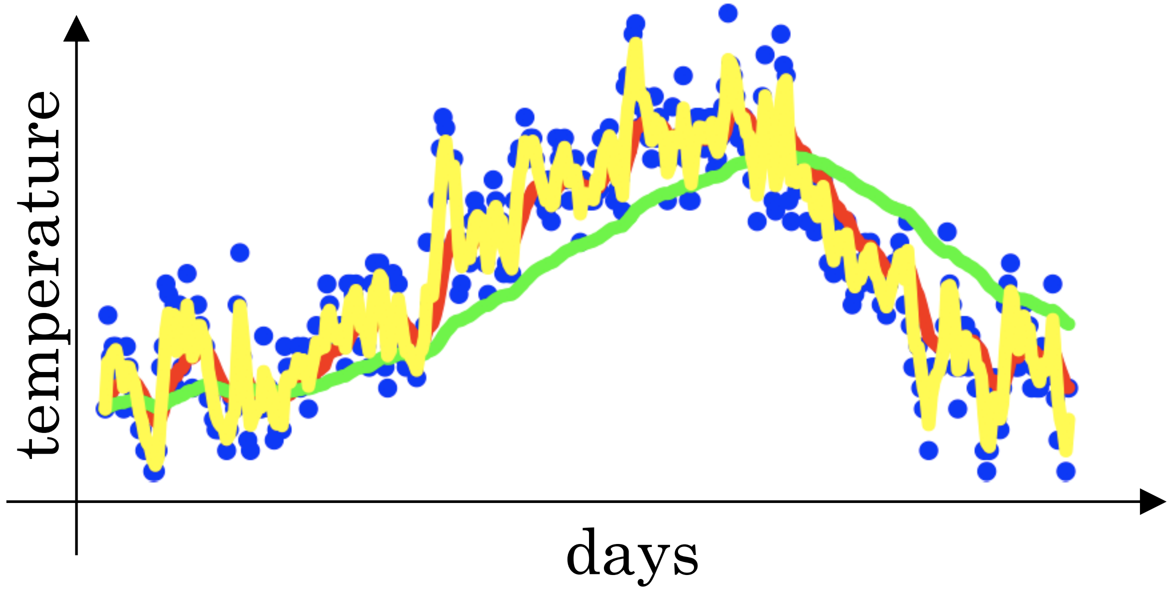
$\beta = 0.98$: ≈ 50 days

$\beta = 0.5$: ≈ 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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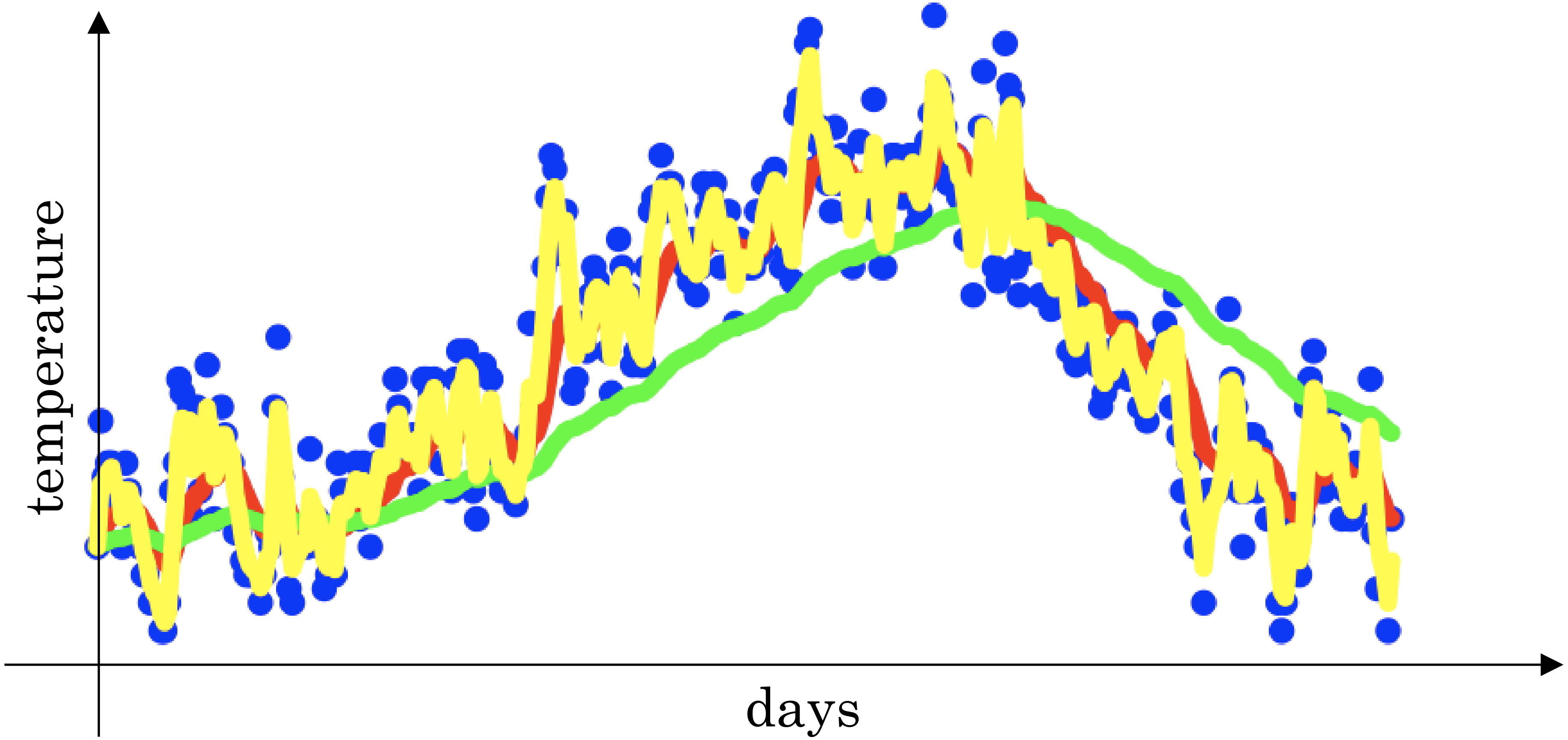
Optimization Algorithms

Understanding exponentially weighted averages

Exponentially weighted averages

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

$\beta = 0.9$ $\quad 0.98 \quad 0.5$



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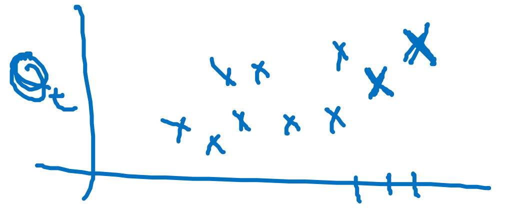
Exponentially weighted averages

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

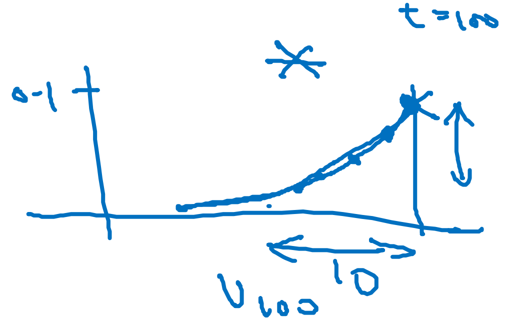


$$v_{100} = 0.9 v_{99} + 0.1 \theta_{100}$$

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

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

...



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

$$\varepsilon = 1-\beta$$

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

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

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

$$+ \dots$$

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

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

$$0.98\ ?$$

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

Implementing exponentially weighted averages

$v_0 = 0$

$v_1 = \beta v_0 + (1-\beta)\,\theta_1$

$v_2 = \beta v_1 + (1-\beta)\,\theta_2$

$v_3 = \beta v_2 + (1-\beta)\,\theta_3$

...

$V_\theta := 0$

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

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

$\vdots$

$\rightarrow V_\theta = 0$

Repeat {

Get next θ_t

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

}

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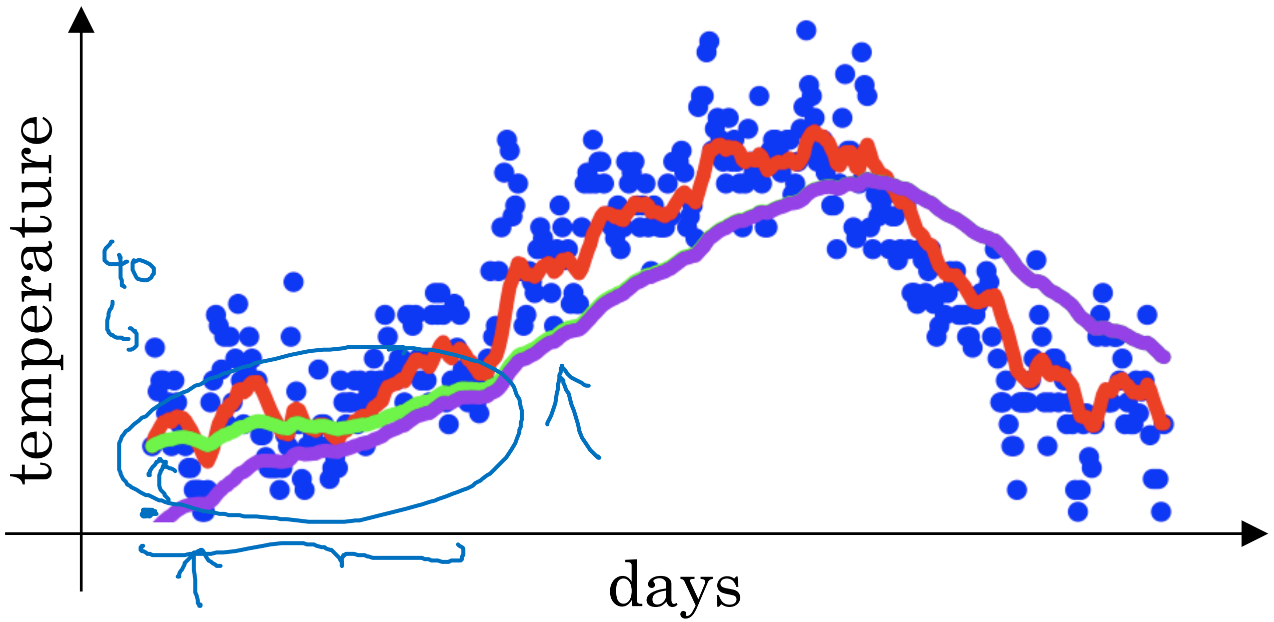
Optimization Algorithms

Bias correction in exponentially weighted average

Bias correction



$\beta = 0.98$

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

$V_0 = 0$

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

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

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

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

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

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

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

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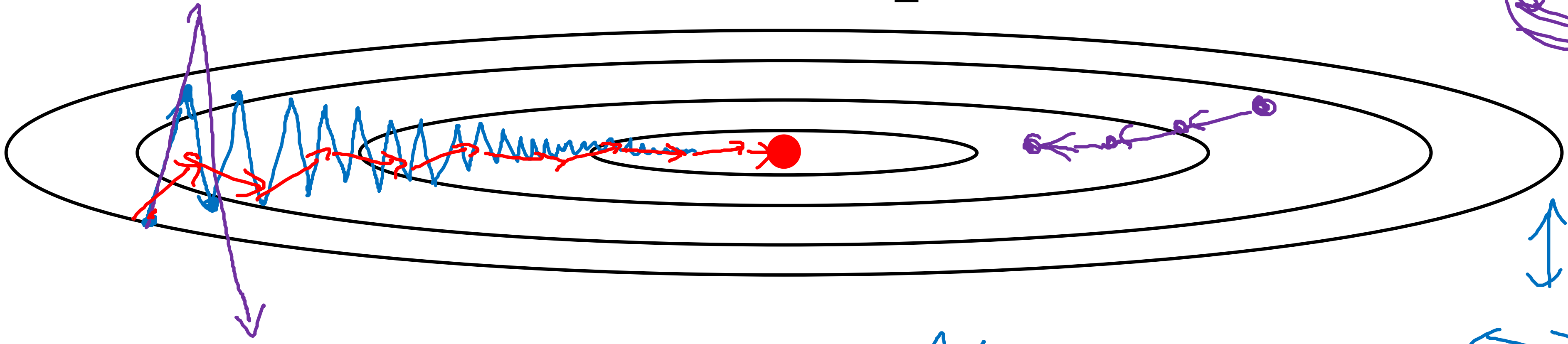
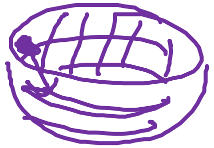
Optimization Algorithms

Gradient descent with momentum

Gradient descent example





$\updownarrow$ slower learning

$\leftrightarrow$ faster learning.

Momentum:

On iteration t:

Compute dW, db on current mini-batch.

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

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

friction, velocity, acceleration

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

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

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Implementation details

$v_{dW} = 0$, $v_{db} = 0$

On iteration t:

Compute dW, db on the current mini-batch

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

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

$$v_{dW} = \beta v_{dW} + dW$$

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

$$\cancel{\frac{v_{dW}}{1-\beta^t}}$$

Hyperparameters: α, β

$\beta = 0.9$

average over last ≈ 10 gradients

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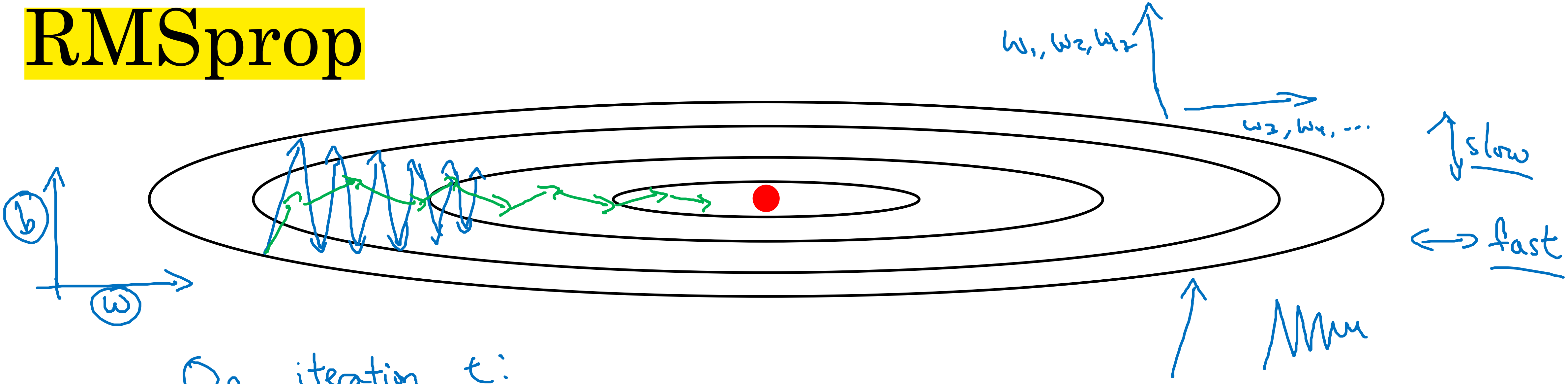
Optimization Algorithms

RMSprop

RMSprop



On iteration t:

Compute dW, db on current mini-batch

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

element-wise

$$\rightarrow S_{db} = \beta_2 S_{db} + (1-\beta_2)\, db^2 \leftarrow \text{large}$$

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

$$\varepsilon = 10^{-8}$$

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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

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

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

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

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

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

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Hyperparameters choice:

→ α : needs to be tune

→ β_1 : 0.9 → $(\underline{dw})$

→ β_2 : 0.999 → $(\underline{dw^2})$

→ ε : 10^{-8}

Adam: Adaptive moment estimation

Adam Coates

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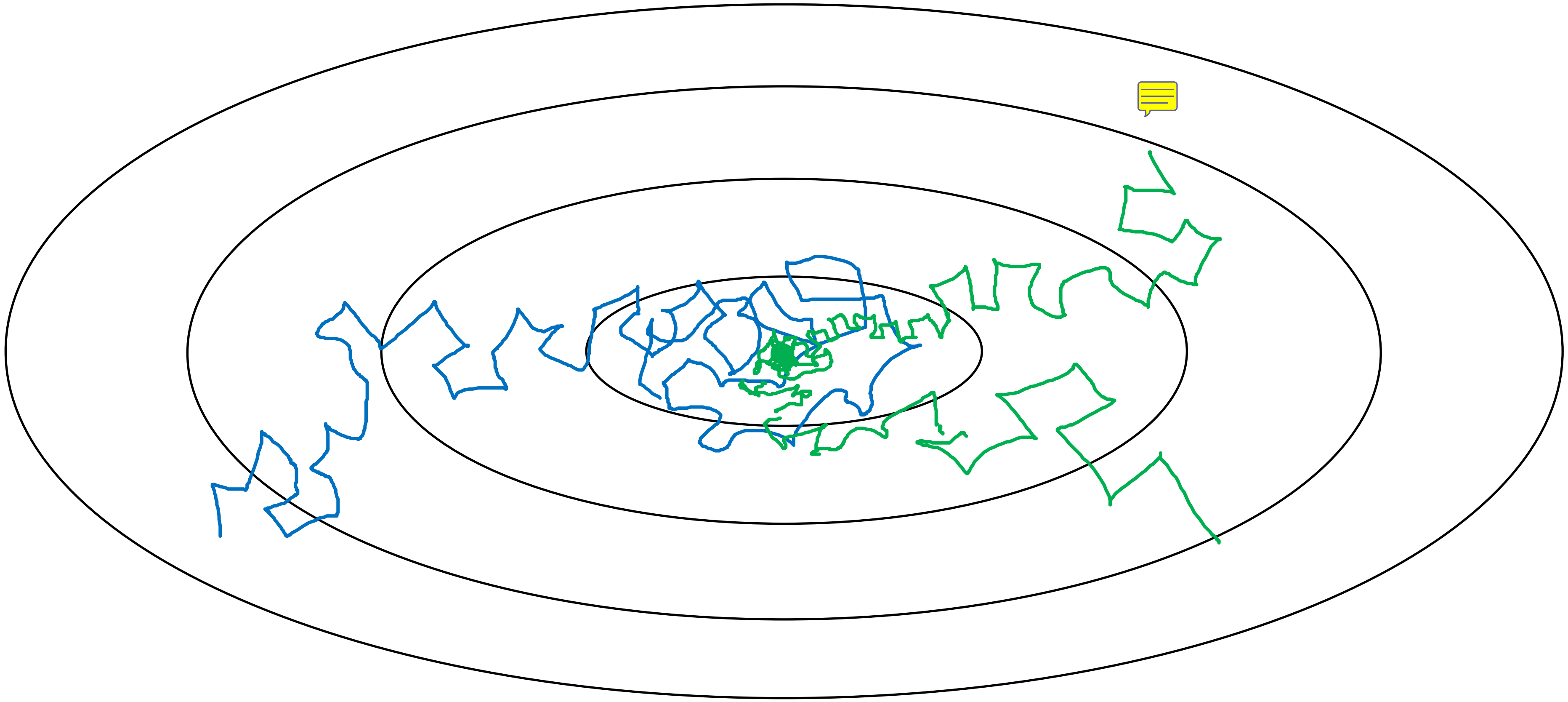
Optimization Algorithms

Learning rate decay

Learning rate decay

Slowly reduce α



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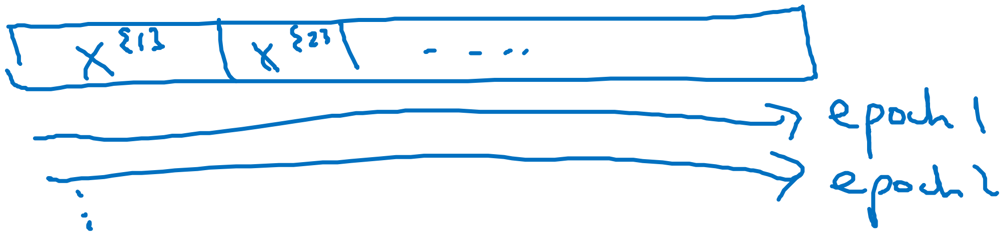
Learning rate decay

1 epoch = 1 pass through data.

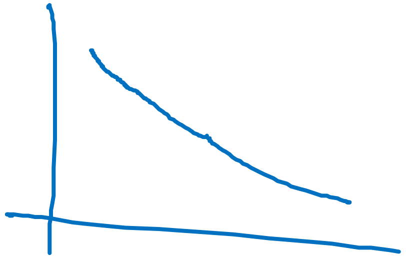


$$\alpha = \frac{1}{1 + \underline{\text{decay-rate}} * \text{epoch-num}} \underline{\alpha_0}$$

Epoch	α
1	0.1
2	0.067
3	0.05
4	0.04
⋮	⋮

$\alpha_0 = 0.2$

decay.rate = 1



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Other learning rate decay methods

formula

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

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

discrete staircase

Manual decay.

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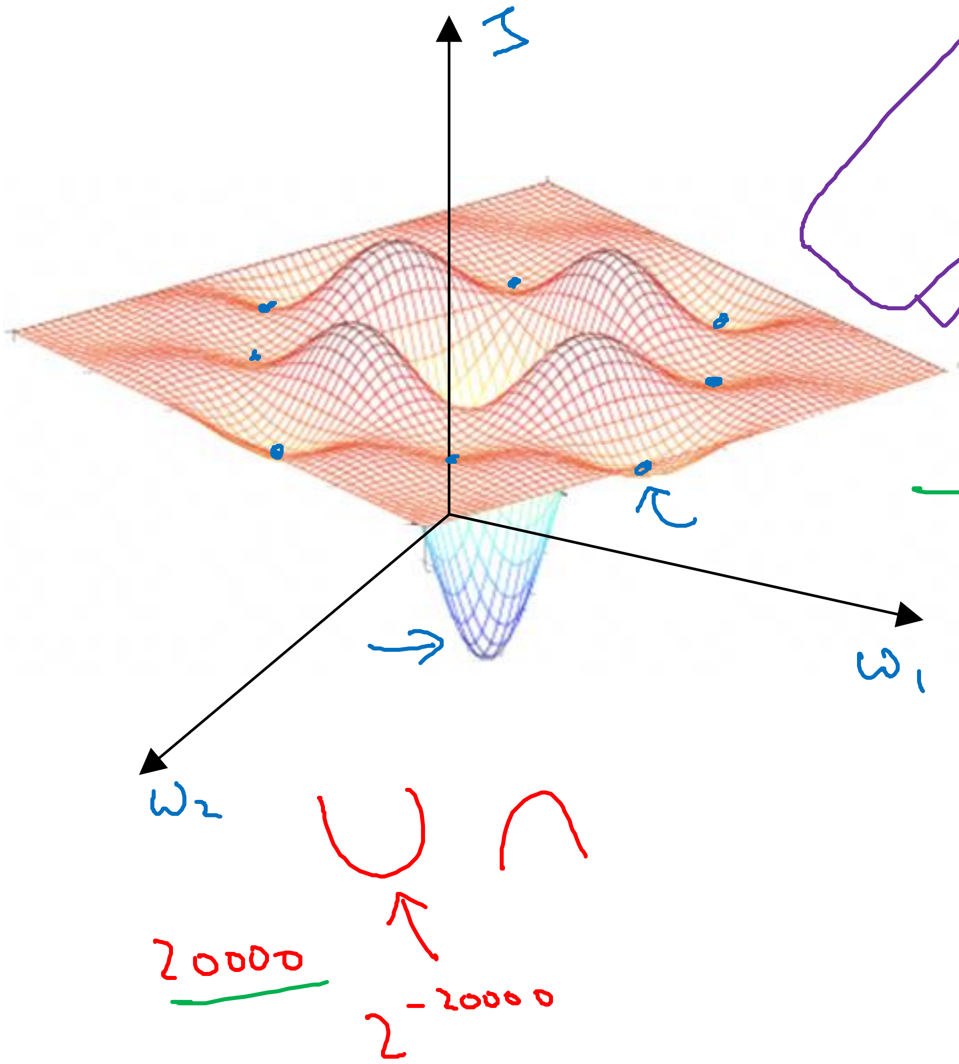
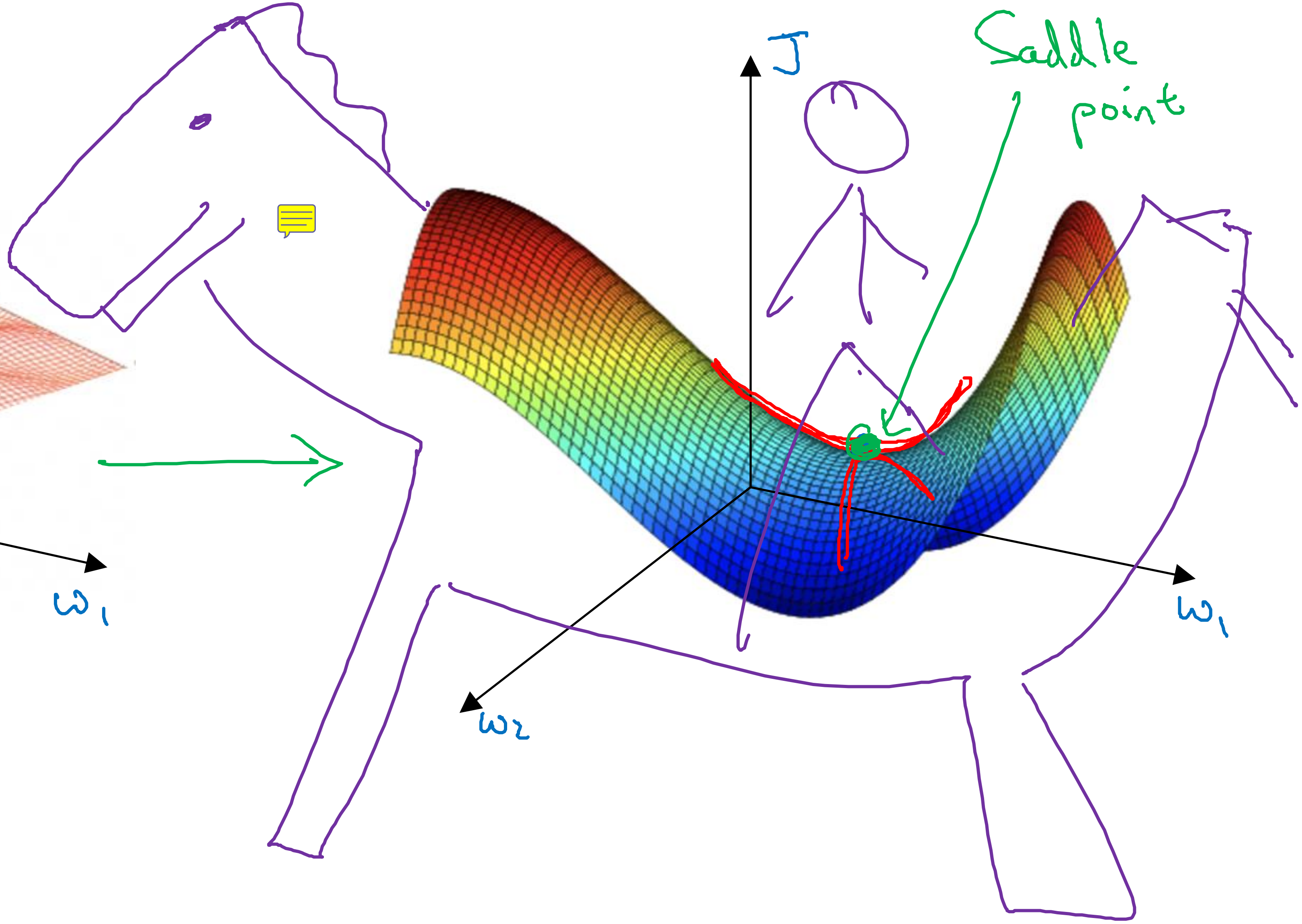
Optimization Algorithms

The problem of local optima

Local optima in neural networks





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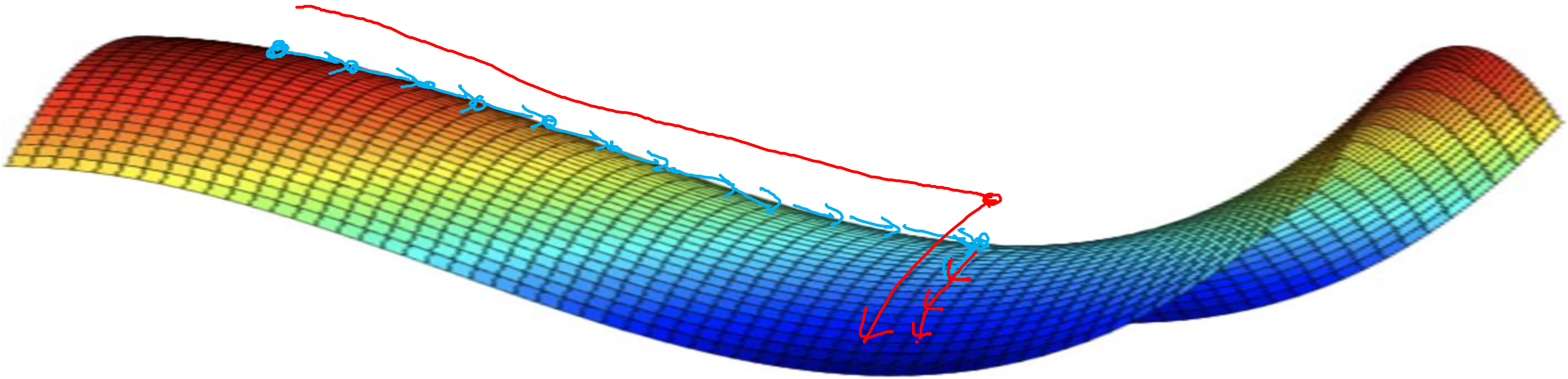
Problem of plateaus



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