Regularization Techniques for Deep Learning

Materials from

- Intel Deep Learning https://www.intel.com/content/www/us/en/developer/learn/course-deep-learning.html
- Improving Deep Neural Networks https://www.deeplearning.ai/

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Regularizing Neural Networks

We have various techniques to "regularize" neural networks – that is, to reduce overfitting

- **Regularization Penalty**: Add penalties (e.g., L1, L2) to the cost function.
- **Dropout**: Randomly deactivate neurons during training.
- **Early Stopping**: Halt training when performance stops improving on validation data.
- **Stochastic/Mini-Batch Gradient Descent**: Adds implicit regularization through noise.

  by introducing noise into the optimization process, stochastic or mini-batch gradient descent can prevent the model from overfitting to training data by promoting generalization, acting as a form of implicit regularization

Penalized Cost function

- One option is to explicitly add a penalty to the loss function for large weights.
- Analogous to the approach used in **Ridge Regression** (L2 regularization).

$$J = \frac{1}{2n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 + \lambda \sum_{j=1}^{m} W_i^2$$

- Can be applied in a similar manner to other loss functions, e.g. Categorical Cross Entropy

$$J = -\frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{K} y_{i,k} \log(\hat{y}_{i,k}) + \lambda \sum_{j=1}^{m} W_j^2$$

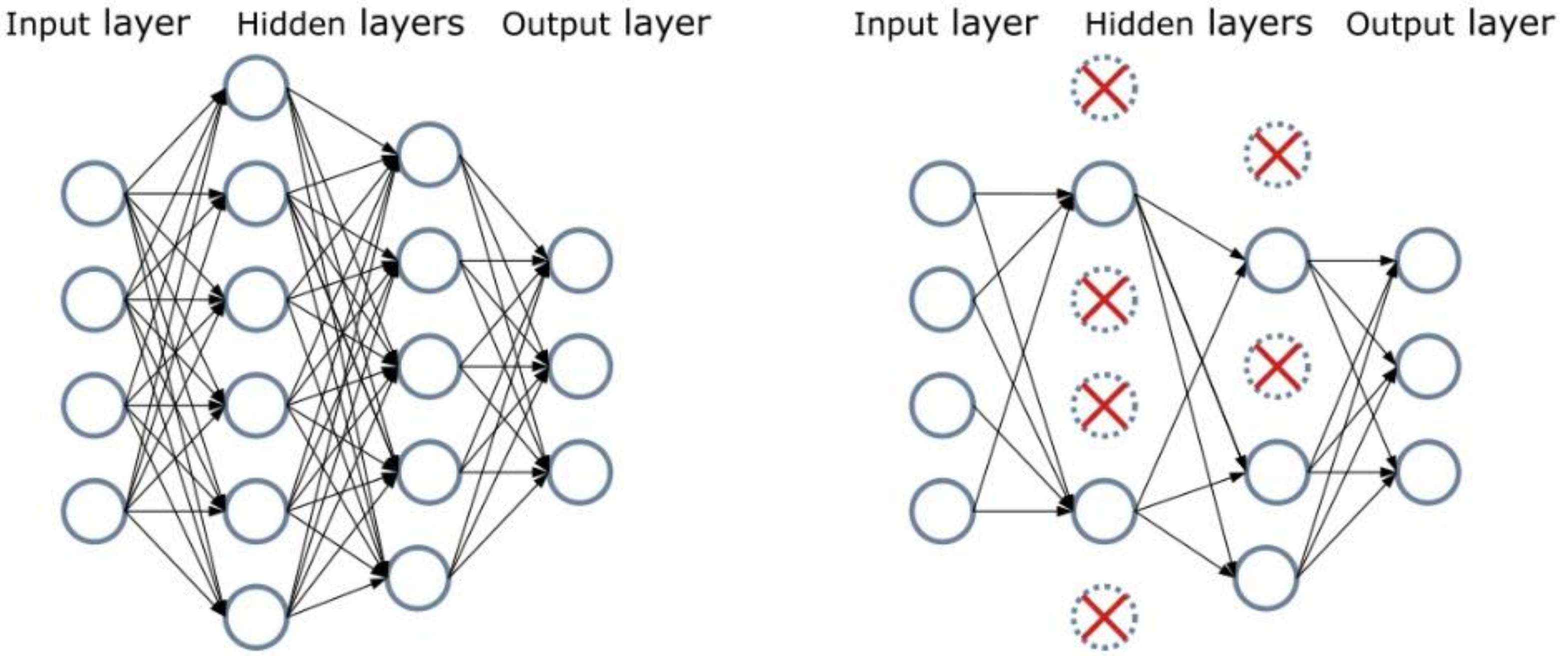
Dropout

- Dropout is a mechanism where we randomly deactivate a subset of neurons in the hidden layers during each training iteration

- This prevents the neural network from relying too much on individual pathways, making it more “robust”

- At test time, we rescale neuron weights to account for the percentage of time they were active during training

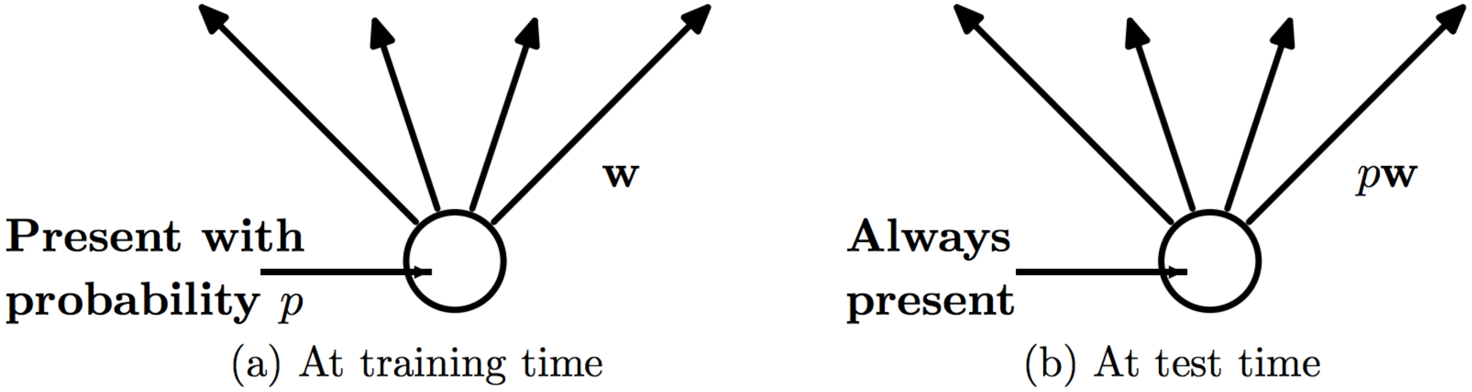
Dropout - Visualization



(a) Standard Neural Net (b) After applying dropout.

Dropout - Visualization

- If the neuron was present with probability *p*, at test time we scale the outbound weights by a factor of *p*.



Dropout – Inverted Dropout Implementation

- We typically implement dropout using inverted dropout because it simplifies the computation during inference (test time).
- If dropout = 0.2, then keep_prop = 1 – dropout = 1 – 0.2 = 0.8
- In inverted dropout, the activations are scaled during training by 1/keep_prob.
- This ensures that the output distributions remain consistent between training and testing, so no scaling is needed during inference.
- Scaling during training avoids extra operations at test time, making the implementation cleaner and more efficient.

Dropout – Inverted Dropout Implementation

considering at layer $\ell = 3$, dropout = 0.2 → keep_prop = 0.8

$$\mathrm{d}^{[3]} = \mathrm{random}\left(\mathrm{a}^{[3]}.\mathrm{shape}[0]\right) < \mathrm{keep\_prob}$$

$$a^{[3]} = a^{[3]} \cdot d^{[3]}$$

$$a^{[3]} = \frac{a^{[3]}}{keep\_prob}$$

$$z^{[4]} = W^{[4]}a^{[3]} + b^{[4]}$$

- The activations $a^{[3]}$ are scaled by $\frac{1}{keep\_prob} = \frac{1}{0.8}$ during training.
- This scaling compensates for the 20% of neurons that are randomly dropped out ($1 - \mathrm{keep\_prob} = 0.2$).
- By scaling $a^{[3]}$, the expected value of $z^{[4]}$ remains consistent with the scenario where no dropout occurs. This ensures that the network behaves similarly during inference (test time) without additional adjustments.

Early Stopping

- A heuristic regularization method to prevent overfitting.
- Stop training when validation performance stops improving.

- Example:
  - Check validation loss every 10 epochs.
  - If the loss increases, stop training and use the model from the best epoch.

Optimizers

- We have considered approaches to gradient descent which vary the number of data points involved in a step.
- However, they have all used the standard update formula:

$$\mathrm{W} := W - \alpha \cdot \nabla J$$

- There are several variants to updating the weights which give better performance in practice.
- These successive “tweaks” each attempt to improve on the previous idea.
- The resulting (often complicated) methods are referred to as “optimizers”.

Exponentially Weighted Averages

$\theta_1 = 40°F$ 4°C ←

$\theta_2 = 49°F$ 9°C

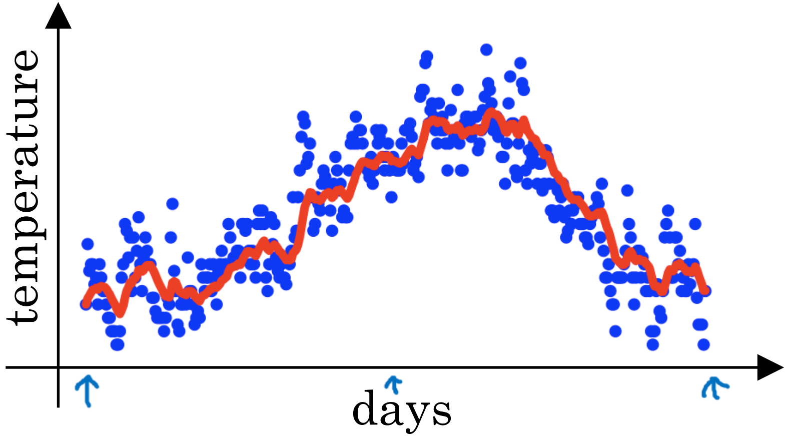
$\theta_3 = 45°F$ ⋮

⋮

$\theta_{180} = 60°F$ 15°C

$\theta_{181} = 56°F$ ⋮

⋮



$V_0 = 0$

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

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

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

⋮

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

Andrew Ng

Exponentially weighted averages

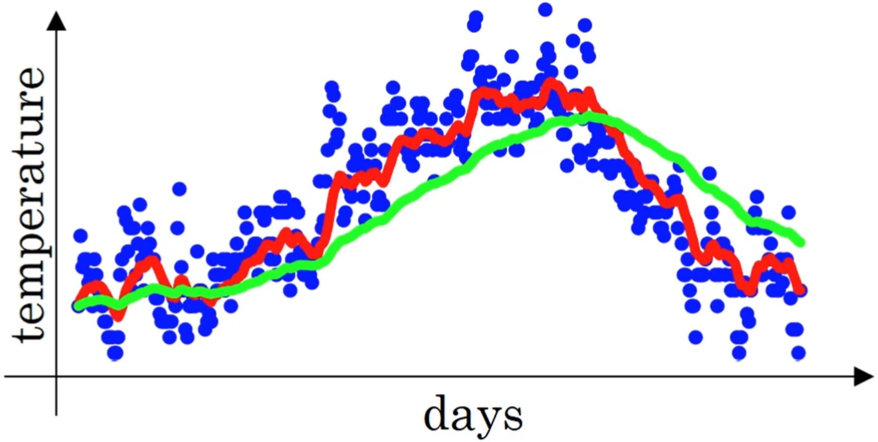
$$V_t = \beta V_{t-1} + (1-\beta)\theta_t$$

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

$\beta = 0.98$: ≈ 50 days

V_t as approximately average over $\approx \frac{1}{1-\beta}$ days' temperature.

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



Andrew Ng

Exponentially weighted averages

moving

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

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

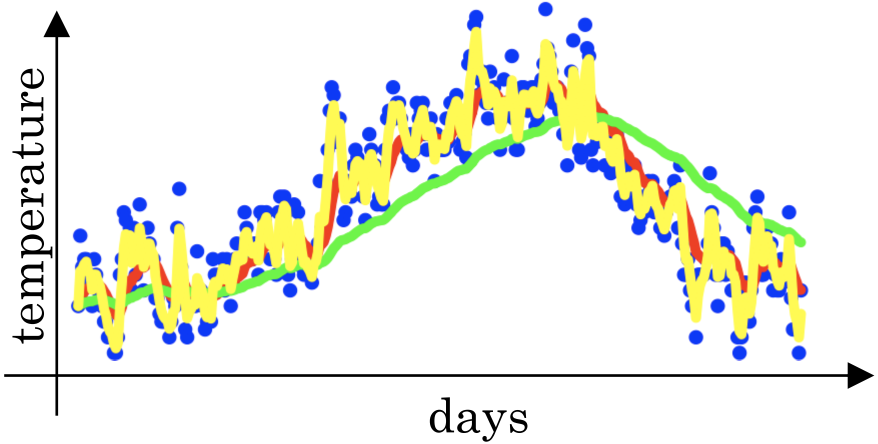
$\beta = 0.98$: ≈ 50 days

$\beta = 0.5$: ≈ 2 days

V_t as approximately average over

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

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



Andrew Ng

Momentum

- Idea: Only change direction slightly with each step to stabilize updates.
- Use a "running average" of previous step directions to smooth out variations in gradients.

$$v_{\mathrm{t}} = \beta \cdot v_{t-1} + (1-\beta) \cdot \nabla J$$

$$\mathrm{W} = W - \alpha \cdot v_t$$

- Here, β is referred to as the "momentum". It is generally given a value <1 (e.g., 0.9 is a common value)

Momentum

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- Use a "running average" of previous step directions to smooth out variations in gradients.

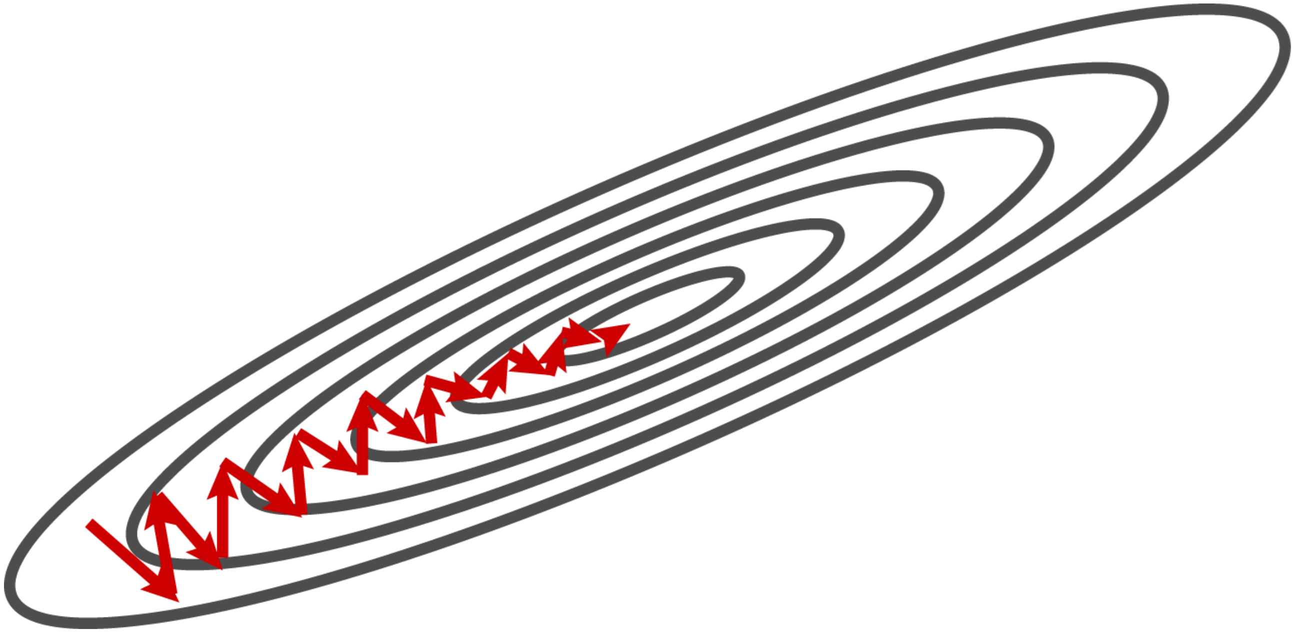
$$v_t = \beta \cdot v_{t-1} + (\cancel{1 - \beta}) \cdot \nabla J$$

often omitted in literatures

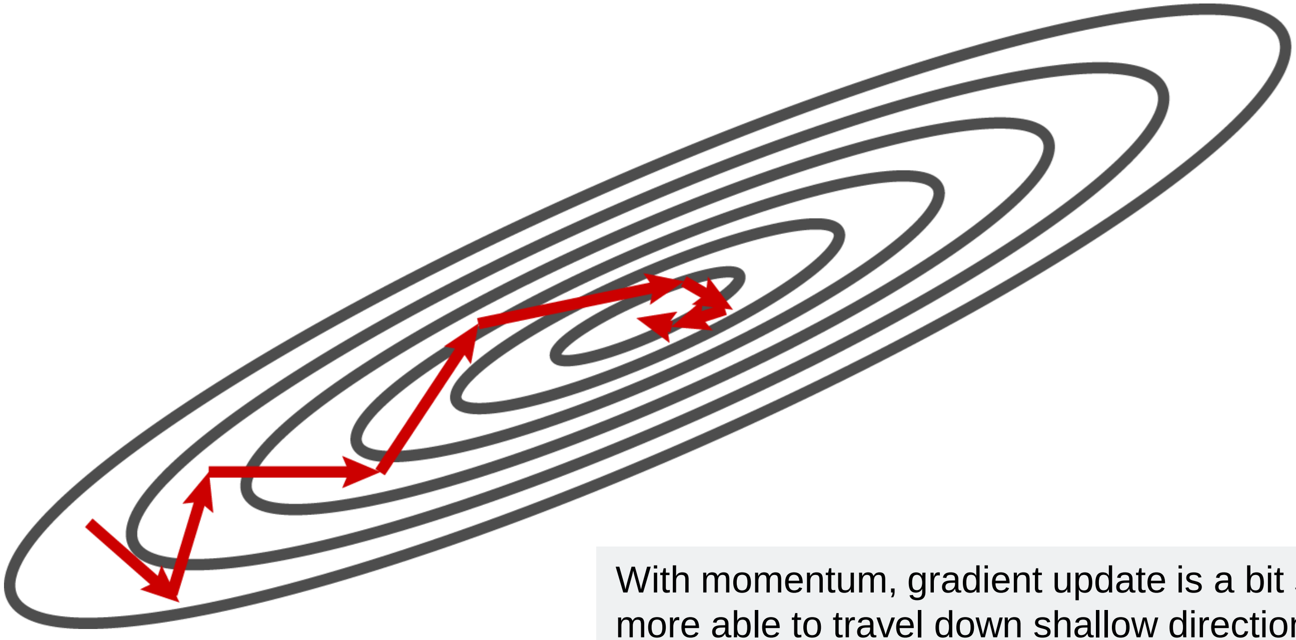
$$W = W - \alpha \cdot v_t$$

- Here, β is referred to as the "momentum". It is generally given a value <1 (e.g., 0.9 is a common value)

Gradient Descent vs Momentum



Gradient Descent vs Momentum



With momentum, gradient update is a bit smoother and more able to travel down shallow directions.

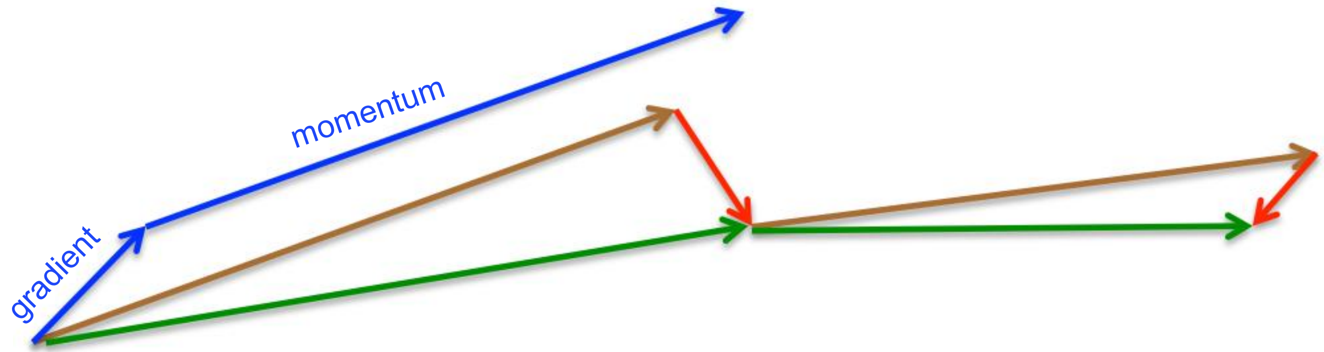
Nesterov Momentum

- Idea: Control "overshooting" by anticipating the next position (lookahead).
- Lookahead Concept: Ensures smoother and more accurate updates by accounting for the momentum's effect before applying the gradient.
- Apply the gradient to the "lookahead" position rather than the current position.

$$v_t = \beta \cdot v_{t-1} + \alpha \, \nabla J(\overbrace{W - \beta \cdot v_{t-1}}^{\text{lookahead}})$$

$$\mathrm{W} = W - v_t$$

Nesterov Momentum



Momentum Vector

Nesterov steps

Gradient/correction

Standard momentum steps

AdaGrad (Adaptive Gradient Optimizer)

- Idea: Scale updates for each weight independently by normalizing with past gradients.
- Divide new updates by factor of previous sum

$$W = W - \frac{\alpha}{\sqrt{G_t + \epsilon}} \nabla J \qquad G_t = G_{t-1} + (\nabla J)^2$$

- Instead of a constant learning rate, the effective learning rate is then divided by the square root of the sum of each component separately.
- Weights with **larger gradients** get **lower learning rates**, while those with smaller gradients get **higher learning rates.**
- However, the **aggressive decay** in the learning rate can slow down convergence, especially in later stages of training.

RMSProp (Root Mean Square Propagation)

- Idea: Similar to Adagrad, but **decays older gradients** exponentially to prioritize recent updates, rather than using the sum of previous gradients
- Adapts learning rates to recent gradient trends, making it more robust to shifts in the shape of the loss function, such as steep valleys.
- Suppresses learning rates for weights with frequent large gradients, helping stabilize training.

$$W = W - \frac{\alpha}{\sqrt{S_t} + \epsilon} \nabla J$$

$$S_t = \beta\, S_{t-1} + (1-\beta)(\nabla J)^2$$

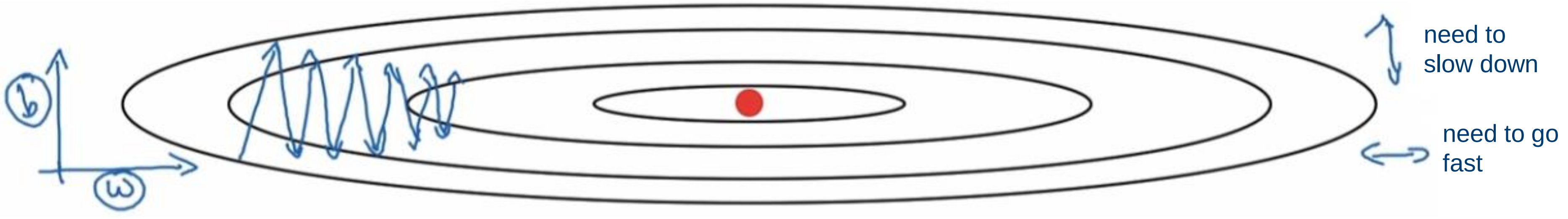
RMSProp (Case Study)

$$S_{dW} = \beta\, S_{dW_{prev}} + (1-\beta)(dW)^2$$

$$S_{db} = \beta\, S_{db_{prev}} + (1-\beta)(db)^2$$

$$W = W - \alpha \frac{dW}{\sqrt{S_{dW}} + \epsilon}$$

$$b = b - \alpha \frac{db}{\sqrt{S_{db}} + \epsilon}$$



Adam (Adaptive Moment Estimation)

- Idea: blending between momentum and RMSprop.
- For iteration t:

$$\mathrm{V_{dW}} = \beta_1 \mathrm{V}_{\mathrm{dW}_{prev}} + (1-\beta_1)\mathrm{dW} \qquad \mathrm{S_{dW}} = \beta_2 \mathrm{S}_{\mathrm{dW}_{prev}} + (1-\beta_2)(\mathrm{dW})^2$$

$$\hat{\mathrm{V}}_{\mathrm{dW}} = \frac{\mathrm{V_{dW}}}{1-\beta_1^t} \qquad \hat{\mathrm{S}}_{\mathrm{dW}} = \frac{\mathrm{S_{dW}}}{1-\beta_2^t}$$

$$W := W - \alpha \frac{\hat{\mathrm{V}}_{\mathrm{dW}}}{\sqrt{\hat{\mathrm{S}}_{\mathrm{dW}}} + \epsilon}$$

Which one should I use?

- **RMSProp** and **Adam** are widely used and effective for most problems.
- The best choice depends on the specific problem and dataset, and it is often hard to predict in advance.
- Optimization algorithm selection remains an **active area of research and experimentation.**

Software