STOCHASTIC OPTIMIZATION FOR LARGE SCALE ML

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MUCH OF ML IS OPTIMIZATION

Linear Classification

$$\arg\min_{w} \sum_{i=1}^{n} ||w||^2 + C \sum_{i=1}^{n} \xi_i$$
$$\text{s.t. } 1 - y_i x_i^T w \leq \xi_i$$
$$\xi_i \geq 0$$

Maximum Likelihood

$$\arg\max_{\theta} \sum_{i=1}^{n} \log\ p_\theta(x_i)$$

K-Means

$$\arg \min_{\mu_1,\mu_2,...,\mu_k} J(\mu) = \sum_{j=1}^{k} \sum_{i \in C_j} ||x_i - \mu_j||^2$$

STOCHASTIC OPTIMIZATION

- Goal of machine learning :
  - Minimize expected loss

$$\min_h L(h) = \mathbf{E}\left[\text{loss}(h(x), y)\right]$$

given samples $(x_i, y_i)\ i = 1, 2 ... m$

- This is Stochastic Optimization
  - Assume loss function is convex

BATCH (SUB)GRADIENT DESCENT FOR ML

- Process all examples together in each step

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \left(\frac{1}{n} \sum_{i=1}^{n} \frac{\partial L(w, x_i, y_i)}{\partial w} \right)$$

where L is the regularized loss function

- Entire training set examined at each step
- Very slow when *n* is very large

STOCHASTIC (SUB)GRADIENT DESCENT

- "Optimize" one example at a time
- Choose examples randomly (or reorder and choose in order)
  - Learning representative of example distribution

for $i = 1$ to n:

$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \frac{\partial L(w, x_i, y_i)}{\partial w}$$

where L is the regularized loss function

STOCHASTIC (SUB)GRADIENT DESCENT

for $i = 1$ to n:

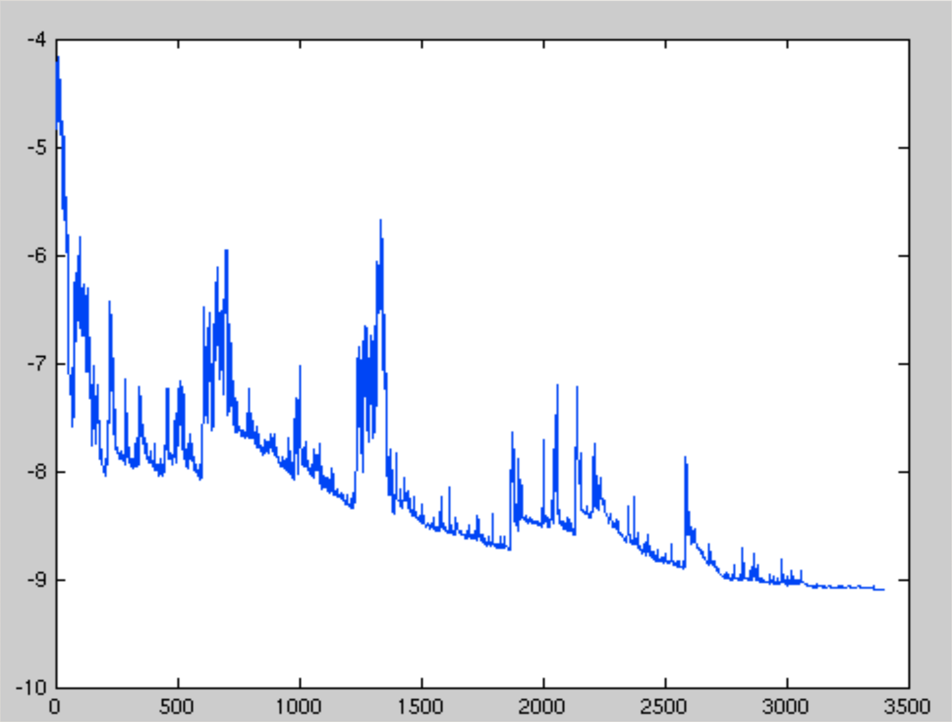
$$w^{(k+1)} \leftarrow w^{(k)} - \eta_t \frac{\partial L(w, x_i, y_i)}{\partial w}$$

where L is the regularized loss function

- Equivalent to online learning (the weight vector *w* changes with every example)
- Convergence guaranteed for convex functions (to local minimum)

SGD CONVERGENCE

Objective function value



Iterations / updates

Objective function oscillates over the iterations.

Not a "Descent Method"

Maintain the **running minimum** loss and corresponding model parameters.

CONVERGENCE OF SGD

- Given dataset $D = \{(x_1, y_1), \ldots, (x_m, y_m)\}$
- Loss function: $L(\theta, D) = \frac{1}{N}\sum_{i=1}^{N} l(\theta; x_i, y_i)$
- For linear models: $l(\theta; x_i, y_i) = l(y_i, \theta^T \phi(x_i))$
- Assumption D is drawn IID from some distribution $\mathcal{P}$.
- Problem:

$$\min_{\theta} L(\theta, D)$$

CONVERGENCE OF SGD

- Input: D
- Output: $\bar{\theta}$

Algorithm:

- Initialize θ^0
- For $t = 1, \ldots, T$

$$\theta^{t+1} = \theta^t - \eta_t \nabla_\theta l(y_t, \theta^T \phi(x_t))$$

- $\bar{\theta} = \frac{\sum_{t=1}^{T} \eta_t \theta^t}{\sum_{t=1}^{T} \eta_t}$.

CONVERGENCE OF SGD

- Expected loss: $s(\theta) = E_{\mathcal{P}}[l(y, \theta^T \phi(x)]$
- Optimal Expected loss: $s^* = s(\theta^*) = \min_{\theta} s(\theta)$
- Convergence:

$$E_{\bar{\theta}}[s(\bar{\theta})] - s^* \leq \frac{R^2 + L^2 \sum_{t=1}^{T} \eta_t^2}{2 \sum_{t=1}^{T} \eta_t}$$

- Where: $R = \|\theta^0 - \theta^*\|$
- $L = \max \nabla l(y, \theta^T \phi(x))$

SGD CONVERGENCE PROOF

- Define $r_t = \|\theta^t - \theta^*\|$ and $g_t = \nabla_\theta l\left(y_t, \theta^T \phi(x_t)\right)$
- $r_{t+1}^2 = r_t^2 + \eta_t^2 \|g_t\|^2 - 2\eta_t(\theta^t - \theta^*)^T g_t$
- Taking expectation w.r.t $\mathcal{P}, \bar{\theta}$ and using $s^* - s(\theta^t) \geq E_P[g_t]^T(\theta^* - \theta^t)$, we get:
  $E_{\bar{\theta}}[r_{t+1}^2 - r_t^2] \leq \eta_t^2 L^2 + 2\eta_t(s^* - E_{\bar{\theta}}[s(\theta^t)])$
- Taking sum over $t = 1, \ldots, T$ and using

$$E_{\bar{\theta}}[r_T^2 - r_0^2] \leq L^2 \sum_{t=0}^{T-1} \eta_t^2 + 2 \sum_{t=0}^{T-1} \eta_t(s^* - E_{\bar{\theta}}[s(\theta^t)])$$

SGD CONVERGENCE PROOF

- Using convexity of s:

$$\left(\sum_{t=0}^{T-1} \eta_t\right) E_{\bar{\theta}}\,[s(\bar{\theta})] \leq E_{\bar{\theta}}[\sum_{t=0}^{T-1} \eta_t s(\theta^t)]$$

- Substituting in the expression from previous slide:

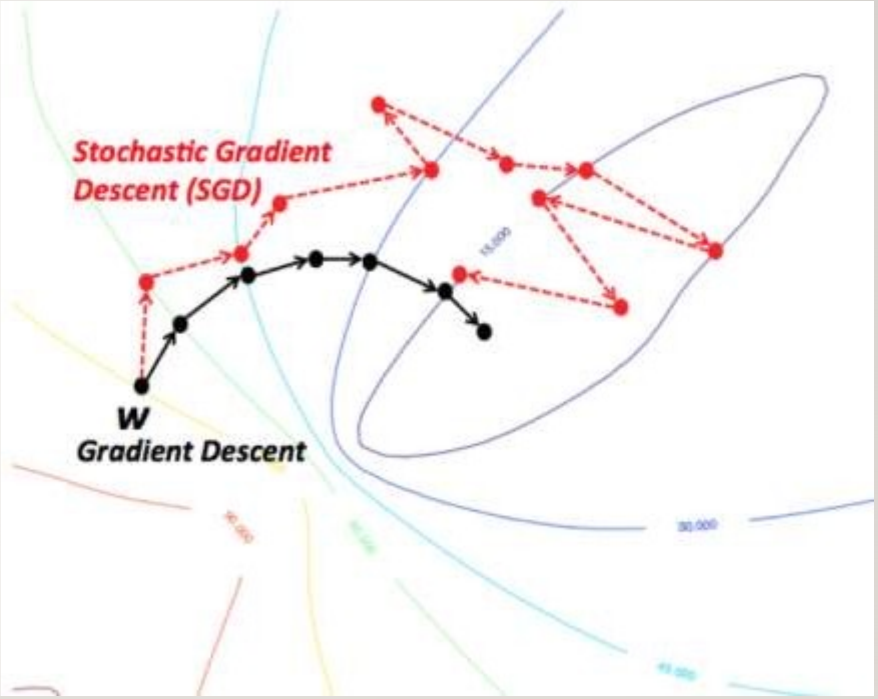
$$E_{\bar{\theta}}[r_T^2 - r_0^2] \leq L^2 \sum_{t=0}^{T-1} \eta_t^2 + 2 \sum_{t=0}^{T-1} \eta_t (s^* - E_{\bar{\theta}}[s(\bar{\theta})])$$

- Rearranging the terms proves the result.

SGD - ISSUES

- Convergence very sensitive to learning rate (η_t)
  (oscillations near solution due to probabilistic nature of sampling)
  - Might need to decrease with time to ensure the algorithm converges eventually

- Basically – SGD good for machine learning with large data sets!



MINI-BATCH SGD

- Stochastic – 1 example per iteration
- Batch – All the examples!
- Mini-batch SGD:
  - Sample *m* examples at each step and perform SGD on them
- Allows for parallelization, but choice of *m* based on heuristics

EXAMPLE: TEXT CATEGORIZATION

- **Example by Leon Bottou:**
  - **Reuters RCV1** document corpus
    - Predict a category of a document
      - One **vs.** the rest classification
  - ***n* = 781,000** training examples (documents)
  - 23,000 test examples
  - ***d* = 50,000** features
    - One feature per word
    - Remove stop-words
    - Remove low frequency words

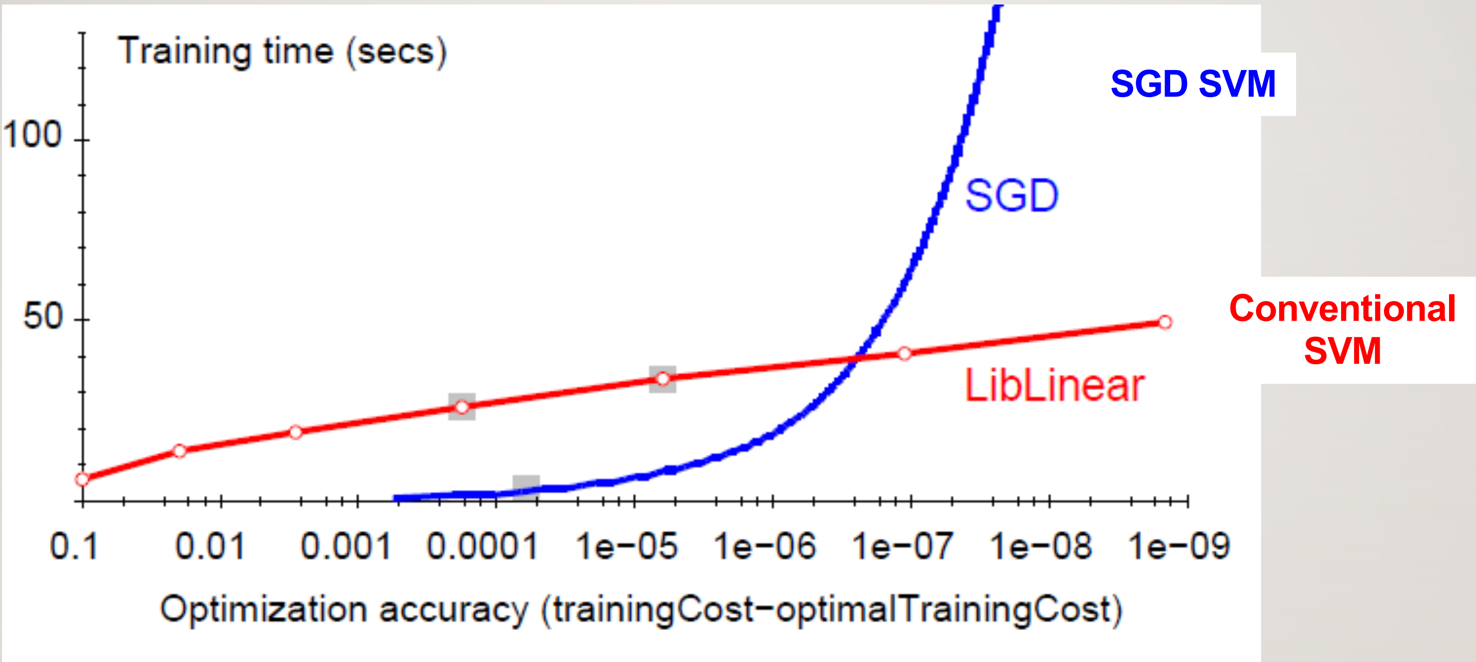
EXAMPLE: TEXT CATEGORIZATION

- **Questions:**
  - **(1)** Is **SGD** successful at minimizing ***f(w,b)***?
  - **(2)** How quickly does **SGD** find the min of ***f(w,b)***?
  - **(3)** What is the error on a test set?

	Training time	*Value of f(w,b)*	*Test error*
Standard SVM	23,642 secs	0.2275	6.02%
"Fast SVM"	66 secs	0.2278	6.03%
SGD SVM	1.4 secs	0.2275	6.02%

(1) SGD-SVM is successful at minimizing the value of ***f(w,b)***
(2) SGD-SVM is super fast
(3) SGD-SVM test set error is comparable

OPTIMIZATION "ACCURACY"



Optimization quality: | *f(w,b)* – *f* (w^{opt},b^{opt}) |

For optimizing *f(w,b) within reasonable* quality *SGD-SVM* is super fast

LEARNING RATE / STEP-SIZE SCHEDULE

- **Need to choose learning rate η and t_0**

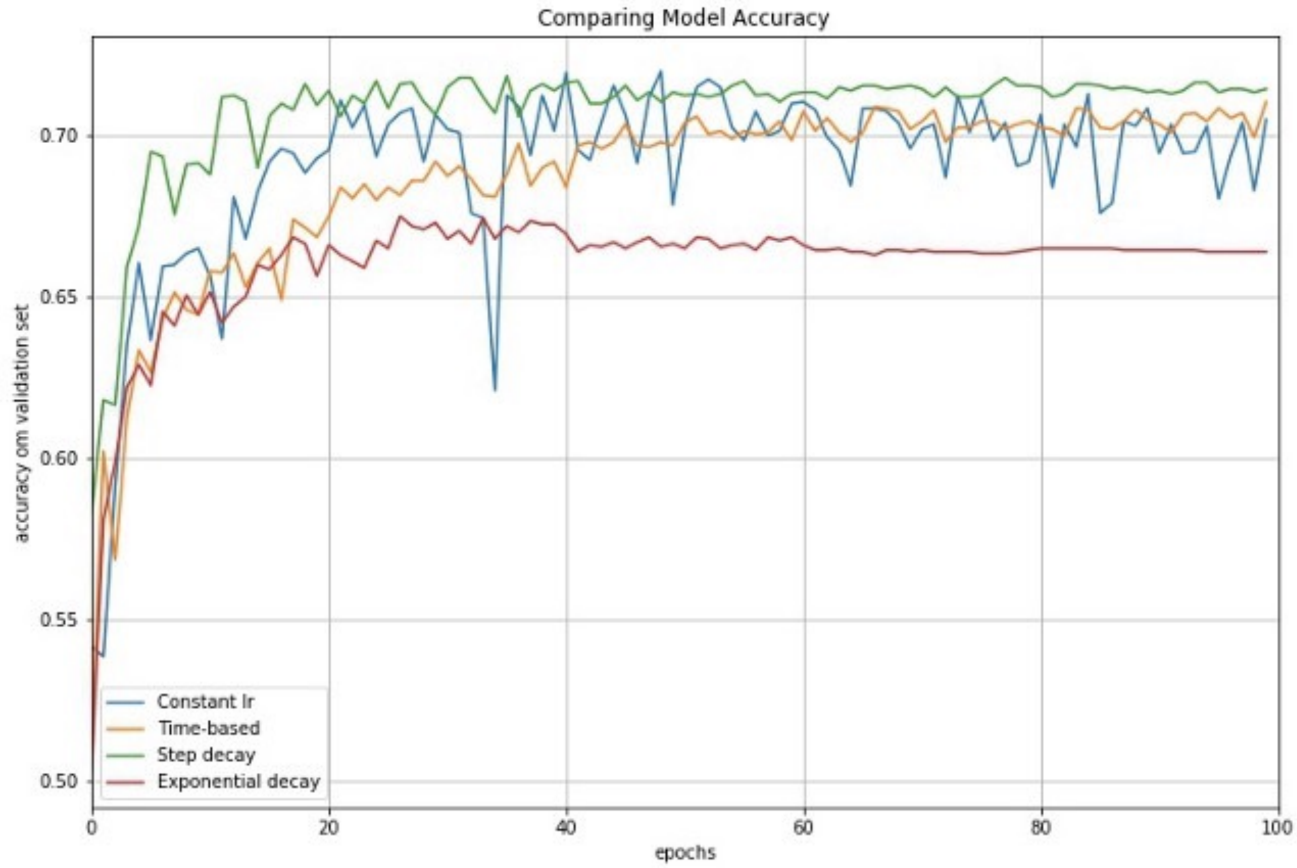
$$w_{t+1} \leftarrow w_t - \frac{\eta_0}{t+t_0}\left(\frac{\partial L(x_i, y_i)}{\partial w}\right); \quad \eta = \frac{\eta_0}{t+t_0}$$

- **Leon suggests:**
  - Choose $\mathbf{t_0}$ so that the expected initial updates are comparable with the expected size of the weights
  - Choose η_0:
    - Select a **small subsample**
    - Try various rates η_0 (e.g., 10, 1, 0.1, 0.01, …)
    - Pick the one that most reduces the cost
    - Use η for next 100k iterations on the full dataset
  - Alternative form:

$$\eta = \frac{\eta_0}{1 + (decay * t)}$$

- Step decay schedule:
  - Drop the learning rate by half every 10 epochs.
    - $\eta = \eta_0 * (drop)^{floor(\frac{t}{t_{drop}})}$

LEARNING RATE COMPARISON



ACCELERATED GRADIENT DESCENT

STOCHASTIC GRADIENT DESCENT

Idea: Perform a parameter update for each training example *x(i)* and label *y(i)*

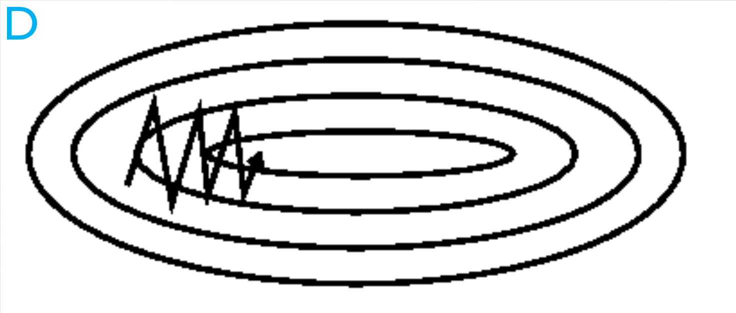
Update: $\theta = \theta - \eta \cdot \nabla_\theta J(\theta; x(i), y(i))$

Performs redundant computations for large datasets

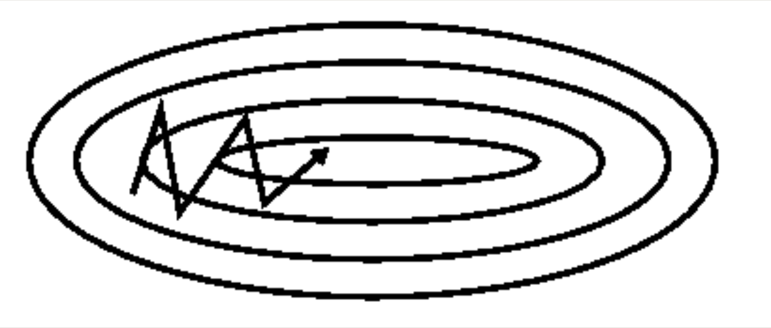
MOMENTUM GRADIENT DESCENT

- Idea: Overcome ravine oscillations by momentum
- Update:
  - $v_t = \gamma v_{t-1} + \eta \cdot \nabla_\theta J(\theta)$
  - $\theta = \theta - v_t$

SGD

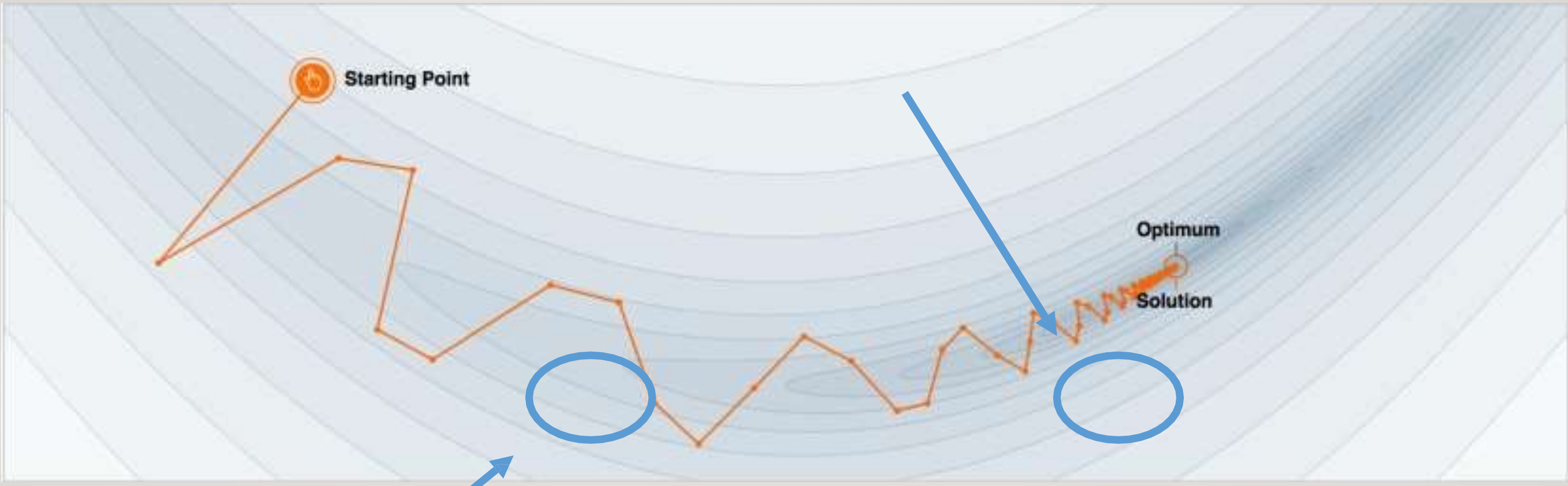


SGD with momentum



WHY MOMENTUM REALLY WORKS

The momentum term **reduces updates for dimensions whose gradients change directions**.



The momentum term **increases for dimensions whose gradients point in the same directions.**

Demo : http://distill.pub/2017/momentum/

NESTEROV ACCELERATED GRADIENT

- However, a ball that rolls down a hill, blindly following the slope, is highly unsatisfactory.
- We would like to have a smarter ball that has a notion of where it is going so that it knows to slow down before the hill slopes up again.
- **Nesterov accelerated gradient** gives us a way of it.

NESTEROV ACCELERATED GRADIENT

$$v_t = \gamma\, v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1})$$
$$\theta = \theta - v_t$$

Approximation of the next position of the parameters(predict)

NESTEROV ACCELERATED GRADIENT

Approximation of the next position of the parameters' gradient(correction)

$$v_t = \gamma\, v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1})$$
$$\theta = \theta - v_t$$

Approximation of the next position of the parameters(predict)

NESTEROV ACCELERATED GRADIENT

Blue line : predict

Red line : correction

Green line :accumulated gradient

Approximation ofthe next position of the parameters' gradient(correction)

$$v_t = \gamma\, v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1})$$
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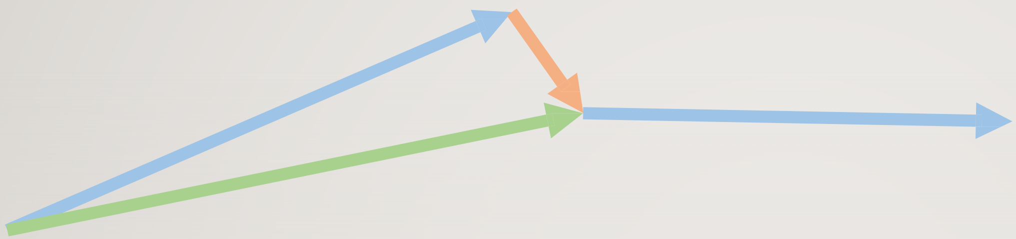

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Approximation of the next position of the parameters(predict)

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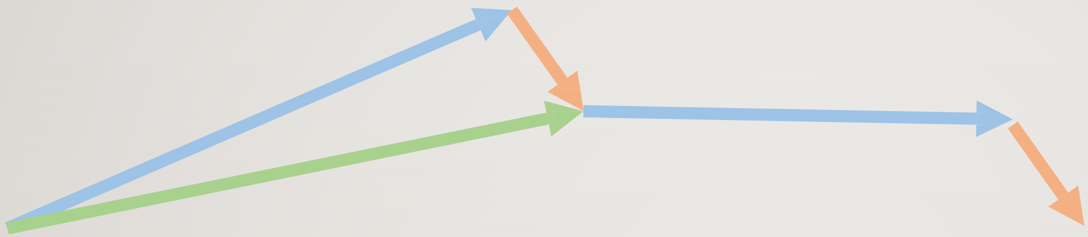

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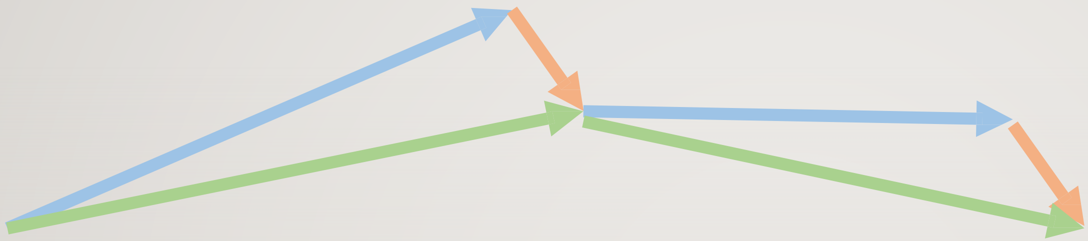

Blue line : predict

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Green line :accumulated gradient

Approximation ofthe next position of the parameters' gradient(correction)

$$v_t = \gamma\, v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1})$$
$$\theta = \theta - v_t$$

Approximation of the next position of the parameters(predict)

NESTEROV ACCELERATED GRADIENT

- This anticipatory update **prevents** us from **going too fast** and **results in increased responsiveness**.
- Now , we can adapt our updates to the slope of our error function and **speed up SGD** in turn.

ADAPTIVE GRADIENTS

- Previous methods :
  - we used the same learning rate $\boldsymbol{\eta}$ for all parameters $\boldsymbol{\theta}$
- Adagrad :
  - It uses a **different learning rate** for every parameter θ_i at every time step t

WHAT'S NEXT ?

- We also want to adapt our updates to each individual parameter to perform larger or smaller updates **depending on their importance**.
  - Adagrad
  - Adadelta
  - RMSprop
  - Adam

ADAGRAD

- Adagrad adapts the learning rate to the parameters
  - Performing larger updates for infrequent
  - Performing smaller updates for frequent parameters.

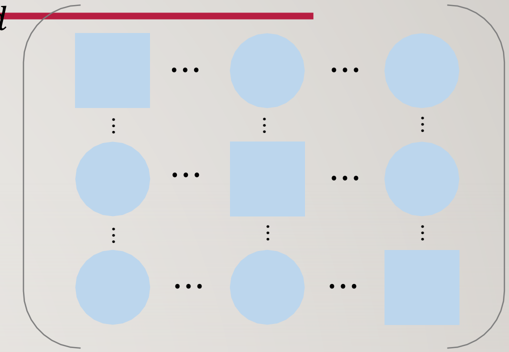
- Ex.
  - Training large-scale neural nets at Google that learned to recognize cats in Youtube videos.

ADAGRAD

SGD

$$\theta_{t+1,i} = \theta_{t,i} - \eta \cdot g_{t,i}$$

$\mathbb{R}^{d\times d}$

$G_t =$ 

Adagrad modifies the general learning rate η based on the past gradients that have been computed for θ_i

Adagrad

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i}$$

$$g_{t,i} = \nabla_\theta J(\theta_i)$$

Vectorize

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t.$$

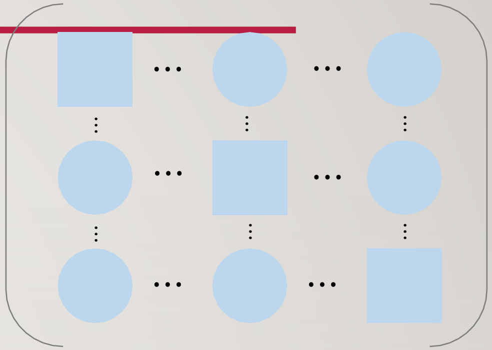
ADAGRAD

SGD

$$\theta_{t+1,i} = \theta_{t,i} - \eta \cdot g_{t,i}$$

$\mathbb{R}^{d \times d}$

$G_t =$



G_t is a diagonal matrix where each diagonal element (i,i) is the sum of the squares of the gradients θ_i up to time step t.

$$G_{t,ii} = \sum_{k=1}^{t} g_{t,i}^2$$

Adagrad

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i}$$

Vectorize

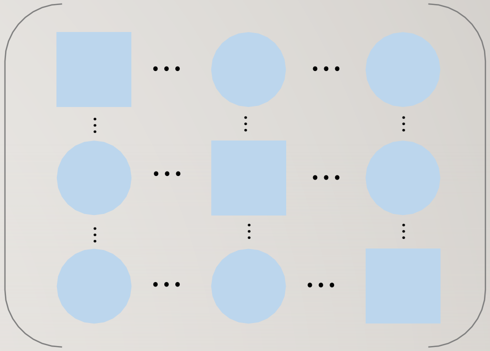
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t.$$

ADAGRAD

SGD

$$\theta_{t+1,i} = \theta_{t,i} - \eta \cdot g_{t,i}$$

$$G_t = \mathbb{R}^{d \times d}$$



ε is a smoothing term that avoids division by zero (usually on the order of 1e − 8).

Adagrad

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i}$$

$$g_{t,i} = \nabla_\theta J(\theta_i)$$

Vectorize

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t.$$

ADAGRAD'S ADVANTAGE

- Advantages :
  - It is well-suited for dealing with sparse data.
  - It greatly improved the robustness of SGD.
  - It eliminates the need to manually tune the learning rate.

ADAGRAD'S DISADVANTAGE

- Disadvantage :
  - Main weakness is its accumulation of the squared gradients in the denominator.

ADAGRAD'S DISADVANTAGE

- The disadvantage causes the learning rate to shrink and become infinitesimally small. The algorithm can no longer acquire additional knowledge.

- The following algorithms aim to resolve this flaw.
  - Adadelta
  - RMSprop
  - Adam

ADADELTA

- The expected square sum of gradients is recursively defined as a decaying average of all past squared gradients.

$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2$$

  - $E[g^2]_t$: The running average at time step t.
  - γ : A fraction similarly to the Momentum term, around 0.9

ADADELTA

Adagrad

$$\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$$

SGD

$$\Delta\theta_t = -\eta \cdot g_{t,i}$$
$$\theta_{t+1} = \theta_t + \Delta\theta_t$$

Adadelta

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

ADADELTA

Adagrad

$$\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$$

SGD

$$\Delta\theta_t = -\eta \cdot g_{t,i}$$
$$\theta_{t+1} = \theta_t + \Delta\theta_t$$

Replace the diagonal matrix G_t with the decaying average over past squared gradients $E[g^2]_t$

Adadelta

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

ADADELTA

Adagrad

$$\Delta\theta_t = -\frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$$

SGD

$$\Delta\theta_t = -\eta \cdot g_{t,i}$$
$$\theta_{t+1} = \theta_t + \Delta\theta_t$$

Replace the diagonal matrix G_t with the decaying average over past squared gradients $E[g^2]_t$

Adadelta

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

Adadelta

$$\Delta\theta_t = -\frac{\eta}{RMS[g]_t} g_t$$

ADADELTA

- The units in this update do not match and the update should have the same hypothetical units as the parameter.
  - As well as in SGD, Momentum, or Adagrad

- To realize this, first defining another exponentially decaying average

$$E[\Delta\theta^2]_t = \gamma E[\Delta\theta^2]_{t-1} + (1-\gamma)\Delta\theta_t^2$$

ADADELTA

$$E[g^2]_t = \gamma E[g^2]_{t-1} + (1-\gamma) g_t^2$$

$$E[\Delta\theta^2]_t = \gamma E[\Delta\theta^2]_{t-1} + (1-\gamma) \Delta\theta_t^2$$

$$RMS[\Delta\theta]_t = \sqrt{E[\Delta\theta^2]_t + \epsilon}$$

Adadelta

$$\Delta\theta_t = -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

Adadelta

$$\Delta\theta_t = -\frac{\eta}{RMS[g]_t} g_t$$

ADADELTA UPDATE RULE

- Replacing the learning rate η in the previous update rule with $RMS[\Delta\theta]_{t-1}$ finally yields the Adadelta update rule:

$$\Delta\theta_t = -\frac{RMS[\Delta\theta]_{t-1}}{RMS[g]_t} g_t$$
$$\theta_{t+1} = \theta_t + \Delta\theta_t$$

- Note : **we do not even need to set a default learning rate**

RMSPROP

RMSprop and Adadelta have both been developed independently around the same time to resolve Adagrad's radically diminishing learning rates.

RMSprop

$$E[g^2]_t = 0.9E[g^2]_{t-1} + 0.1g_t^2$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

RMSPROP

RMSprop as well divides the learning rate by an exponentially decaying average of squared gradients.

RMSprop

$$E[g^2]_t = 0.9E[g^2]_{t-1} + 0.1g_t^2$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} g_t$$

Hinton suggests γ to be set to 0.9, while a good default value for the learning rate η is 0.001.

ADAM

- Adam's feature :
  - Storing an exponentially decaying average of past squared gradients v_t like Adadelta and RMSprop
  - Keeping an exponentially decaying average of past gradients m_t, similar to momentum.

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$

→ The first moment (the mean)

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

→ The second moment (the uncentered variance)

ADAM

- As m_t and v_t are initialized as vectors of 0's, they are biased towards zero.
  - Especially during the initial time steps
  - Especially when the decay rates are small
    - (i.e. β1 and β2 are close to 1).

- Counteracting these biases in Adam

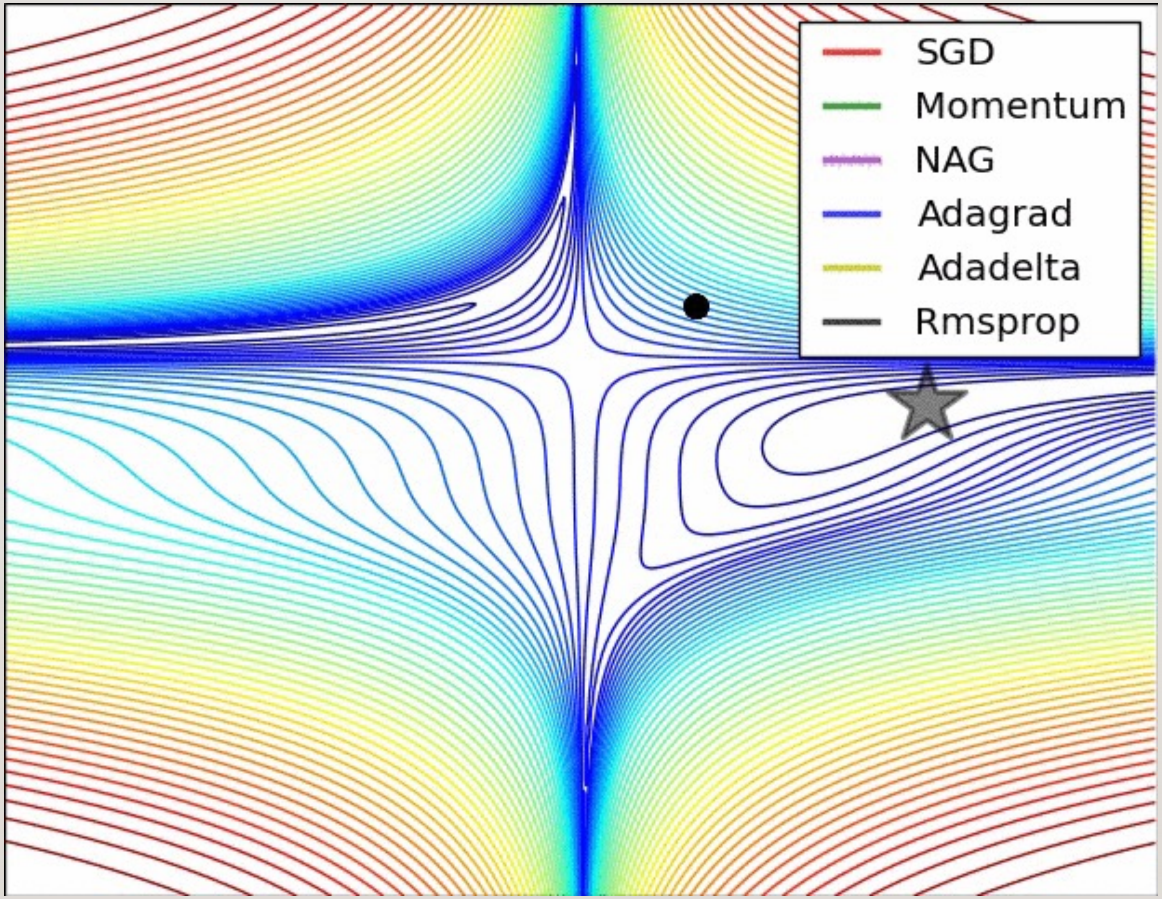
$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$
$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

Adam

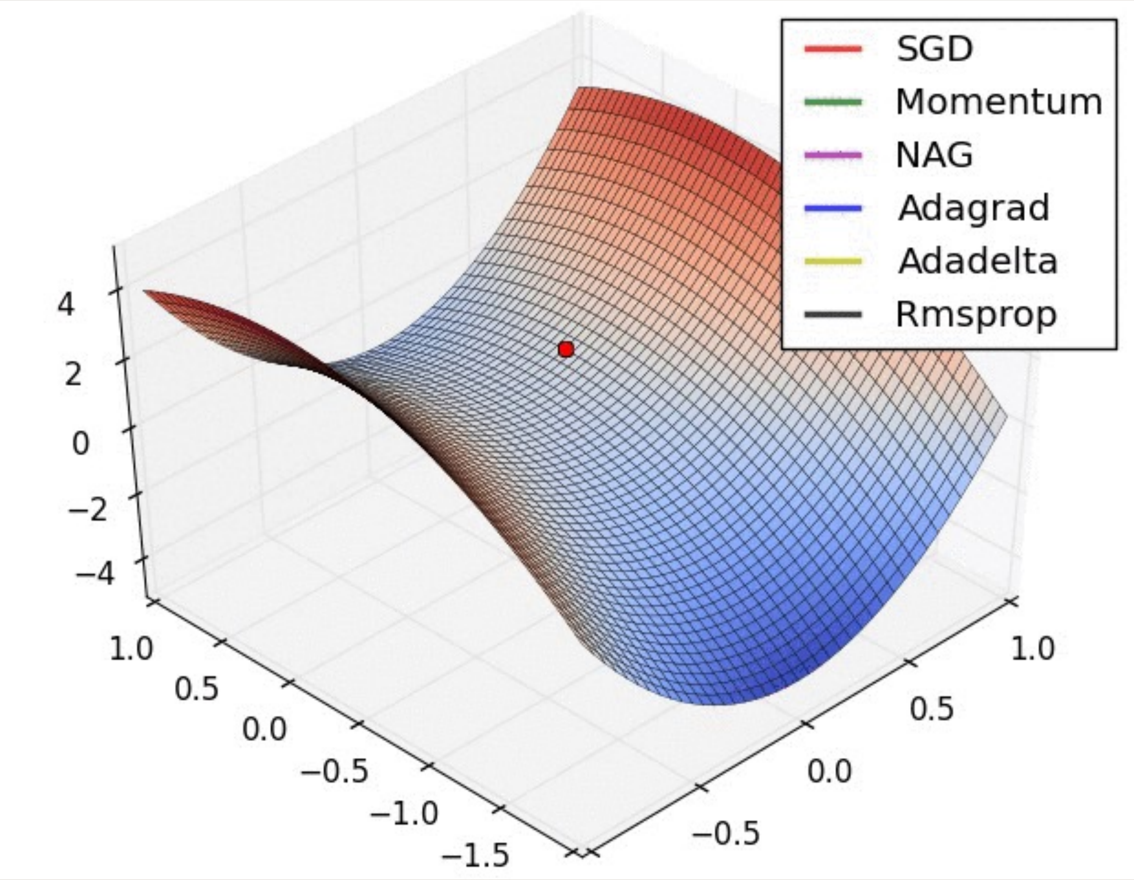
$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$$

Note : default values of 0.9 for β_1, 0.999 for β_2, and 10^{-8} for ε

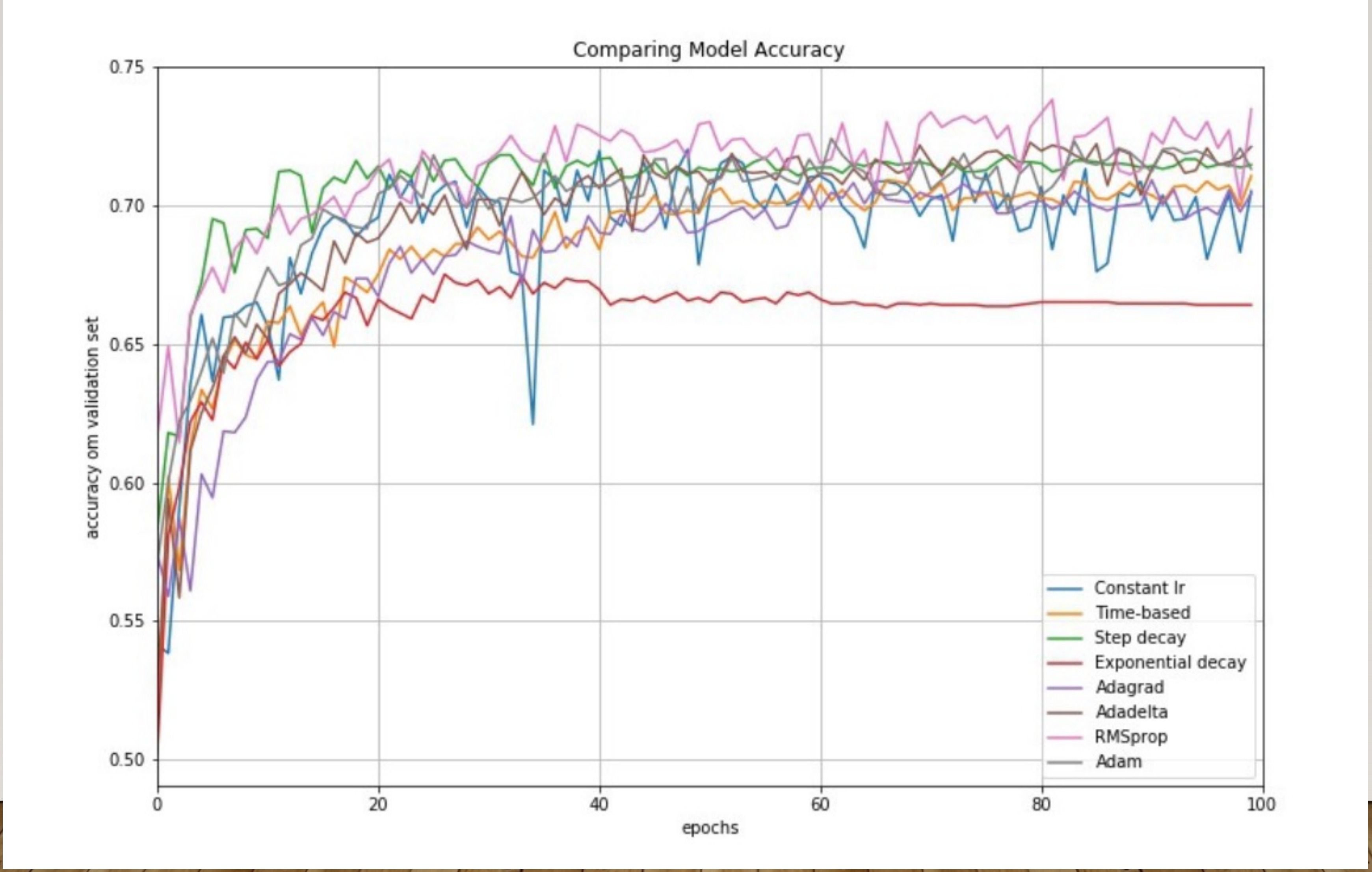
VISUALIZATION



VISUALIZATION



ENHANCEMENTS COMPARISON



SUMMARY

- There are two main ideas at play:
  - Momentum : Provide consistency in update directions by incorporating past update directions.
  - Adaptive gradient : Scale the scale updates to individual variables using the second moment in that direction.
  - This also relates to adaptively altering step length for each direction.

References:

- **SGD convergence** proof: "Confidence level solutions for stochastic programming" by Y. Nesterov, P. Vial, Automatica, 2008.
- **Accelerated SGD:** Ruder, Sebastian. "An overview of gradient descent optimization algorithms." *arXiv preprint arXiv:1609.04747* (2016).
- **First SGD in ML paper**:
  Léon Bottou and Olivier Bousquet: **The Tradeoffs of Large Scale Learning**, *Advances in Neural Information Processing Systems*, 20, MIT Press, Cambridge, MA, 2008.

THANKS

QUESTIONS?

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