Optimization Algorithms in Deep Learning

Stochastic Gradient Descent and ADAM

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ERM Framework for Deep Learning

- Under ERM, given the training data set $\{(\boldsymbol{X}_i, \boldsymbol{Y}_i)\}_{i=1}^n$ and a loss function $\mathcal{L}$, training a deep neural network can be formulated as

$$\hat{f} = \mathrm{argmin}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(f(\boldsymbol{X}_i), \boldsymbol{Y}_i), \tag{1}$$

where

$$\mathcal{F} = \left\{ f : \mathbb{R}^d \to \mathbb{R} : f(\boldsymbol{x}) = \sigma_L(\boldsymbol{W}_L \cdots \sigma_2 \boldsymbol{W}_2(\sigma_1(\boldsymbol{W}_1 \boldsymbol{x}))) \right\}$$

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- Each member in $\mathcal{F}$ is parameterized by weight matrices $\Theta = (\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L)$, so problem (1) is equivalent to

$$\hat{\Theta} = \mathrm{argmin}_{\Theta} \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(f_\Theta(\boldsymbol{X}_i), \boldsymbol{Y}_i).$$

Gradient Descent

- Gradient Descent Updating Scheme:

$$\Theta^{(k+1)} = \Theta^{(k)} - \eta \frac{1}{n} \sum_{i=1}^{n} \nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}_i), \boldsymbol{Y}_i).$$

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- Two natural questions for GD are
  1. When GD converges, does it converge to a local minimum or a saddle point?
  2. How long does it take to converge (i.e. convergence speed)?

A Recap from Calculus – Saddle Points

Let $g : \mathbb{R}^p \to \mathbb{R}$ and our goal is to minimize $g(\boldsymbol{x}) \in C^2$.

- (*2nd Order Necessary Condition*) If $\boldsymbol{x}^*$ is a local minimizer, then
  - $\nabla g(\boldsymbol{x}^*) = 0$. (*1st Order Necessary Condition*)
  - $\nabla^2 g(\boldsymbol{x}^*)$ is positive semi-definite, i.e. $\lambda_{\min}(\nabla^2 g(\boldsymbol{x}^*)) \geq 0$.

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$$\lambda_{\min}(\nabla^2 g(\boldsymbol{x}^*)) \begin{cases} > 0 & \text{local minimum} \\ = 0 & \text{local minimum or non-strict saddle point} \\ < 0 & \text{strict saddle point} \end{cases}$$

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- Strict saddle points require that there is at least one direction along which the curvature is strictly negative.
- In general, distinguishing local minima and non-strict saddle points is NP-hard.

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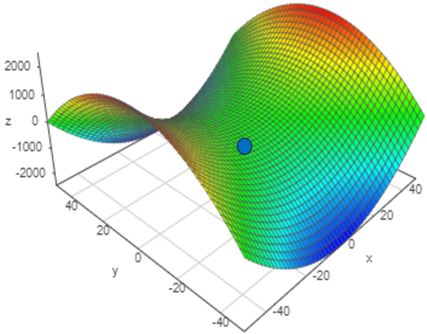
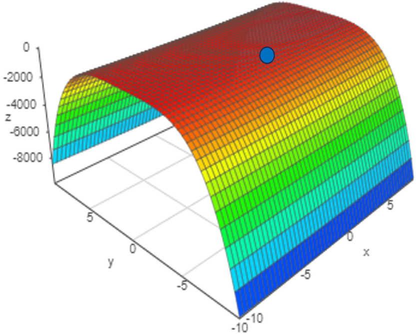


Strict Saddle Point
$f(x, y) = x^2 - y^2$



Non-Strict Saddle Point
$f(x, y) = x^2 - y^4$

Theoretical Guarantee of Gradient Descent (Lee et al. (2016)

Suppose we minimize a differential function $g(\boldsymbol{x})$ via gradient descent:
$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \eta \nabla g(\boldsymbol{x}^{(k)})$

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Theorem

If $g \in C^2$ and $\boldsymbol{x}^*$ is a strit saddle point, then under (A1), (A2) and the assumption that $0 < \eta < 1/\gamma$,

$$\mathbb{P}\left(\lim_k \boldsymbol{x}^{(k)} = \boldsymbol{x}^*\right) = 0.$$

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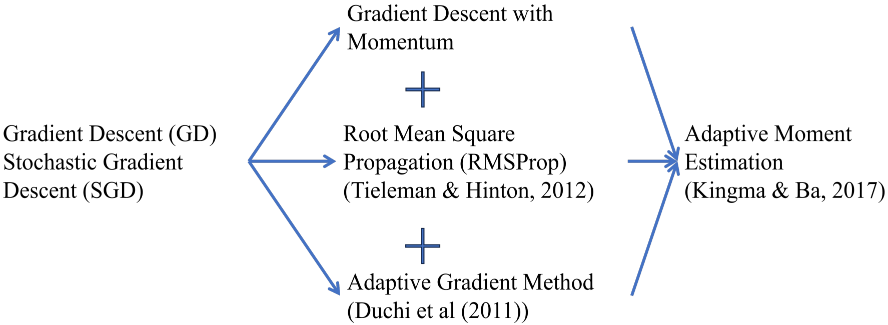
- It may take exponential time to escape (Du et al. 2017).


Gradient Descent (GD)
Stochastic Gradient Descent (SGD)
Gradient Descent with Momentum
Root Mean Square Propagation (RMSProp) (Tieleman & Hinton, 2012)
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Stochastic Gradient Descent (SGD)

- $\Theta^{(k+1)} = \Theta^{(k)} - \eta \frac{1}{n} \sum_{i=1}^{n} \nabla_{\Theta^{(k)}} \mathcal{L}(f_{\Theta}(\boldsymbol{X}_i), \boldsymbol{Y}_i)$.

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- Observation

$$\begin{aligned}
\frac{1}{n} \sum_{i=1}^{n} \nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}_i), \boldsymbol{Y}_i) &= \mathbb{E}_{\mathbb{P}_n}[\nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}), \boldsymbol{Y})] \\
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$$= \int \nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}), \boldsymbol{Y}) d\mathbb{P}_n.$$

- The Idea of SGD is to replace $\mathbb{E}_{\mathbb{P}_n}[\nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}), \boldsymbol{Y})]$ by an unbiased estimator and a typical choice is

$$\frac{1}{B} \sum_{i \in \mathcal{S}_j} \nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}_i), \boldsymbol{Y}_i), \quad j = 1, \ldots, \lceil n/B \rceil.$$

where $\mathcal{S}_j$ is chosen uniformly at random among the set of all subsets of size B from $\{1, \ldots, n\}$.

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  where $\mathcal{S}_j$ is chosen uniformly at random among the set of all subsets of size B from $\{1, \ldots, n\}$.
- In deep learning, SGD refers to the case $B = 1$. For $B > 1$, this is known as the mini-batch gradient descent.

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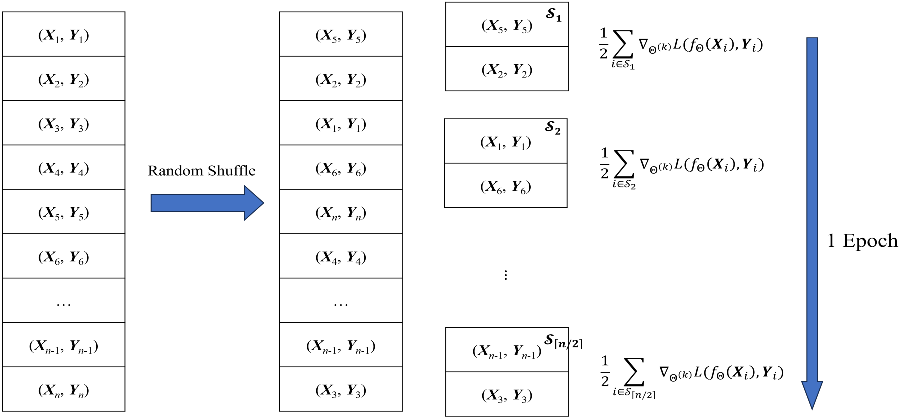

Stochastic Gradient Descent (SGD)

- **Reasons for SGD: memory constraint and faster convergence**.
  - A GPU with memory size 11Gb can only process 512 samples at one time when using AlexNet for ImageNet.
  - SGD is not necessarily faster than GD if all samples can be processed in a single machine in a parallel way, but in the memory-constraint system SGD is often much faster than GD.

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  - SGD is not necessarily faster than GD if all samples can be processed in a single machine in a parallel way, but in the memory-constraint system SGD is often much faster than GD.
- Convergence of SGD:
  - Under some general assumptions, convergence of SGD is guaranteed for SGD if $\eta_k = 1/k^\alpha$ for $\alpha \in (1/2, 1]$.
  - For constant step size, the gradient does not converge to zero. However, nowadays, SGD with a constant learning rate works quite well in many cases. So there is a gap between theory and applications.

GD with Momentum

- $\boldsymbol{p} = m\boldsymbol{v}$. Momentum is a measure of the amount of motion that an object has. An object with a high momentum will be harder to stop or change direction than an object with a low momentum.

GD with Momentum

- GD update: $\Theta^{(k+1)} = \Theta^{(k)} - \eta \frac{1}{n} \sum_{i=1}^{n} \nabla_{\Theta^{(k)}} \mathcal{L}(f_{\Theta}(\boldsymbol{X}_i), \boldsymbol{Y}_i)$.

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- GD with momentum update:
  - Momentum: $m^{(k+1)} = \beta m^{(k)} + (1 - \beta) \frac{1}{n} \sum_{i=1}^{n} \nabla_{\Theta^{(k)}} \mathcal{L}(f_\Theta(\boldsymbol{X}_i), \boldsymbol{Y}_i)$
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- A common choice for β in practice is 0.9.
- GD with momentum almost always works faster than GD. However, this is not true for the naive stochastic version.

Adaptive Gradient Method (AdaGrad), Duchi et al, 2011

- At the k-the iteration, update the parameter as

$$\Theta^{(k+1)} = \Theta^{(k)} - \eta_k \boldsymbol{G}^{(k)^{-1/2}} \boldsymbol{g}^{(k)}, \quad k = 0, 1, 2, ...,$$

where

$$\boldsymbol{g}^{(k)} = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\Theta^{(k)}} \mathcal{L}(f_{\Theta}(\boldsymbol{X}_i), \boldsymbol{Y}_i)$$

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- Caculating $\boldsymbol{G}^{(k)^{-1/2}}$ may be hard. In practice, using $\mathrm{diag}(\boldsymbol{G}^{(k)})^{-1/2}$ works well enough.
- AdaGrad is shown to exhibit a convergence rate similar to SGD for convex problems and non-convex problems. After T iterations, the error is of the order $1/\sqrt{T}$.

Root Mean Squre Propagation (RMSProp), Tieleman & Hinton, 2012

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- RMSProp update:

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- In deep learning, a small number $\epsilon = 10^{-8}$ is often added to each component in $\mathrm{diag}(\boldsymbol{G}^{(k)})$ to reduce numerical instability.

Root Mean Squre Propagation (RMSProp), Tieleman & Hinton, 2012

Theorem

Assume that the empirical risk function is gradient Lipshitz continuous and lower bounded by R^*. Then RMSProp with diminishing step size $\eta_k = \eta_1/\sqrt{k}$ and any $\beta \in (0, 1)$,

$$\min_{k\in(1,T]} \left\|\boldsymbol{g}^{(k)}\right\|_1 \leq \mathcal{O}\left(\frac{\log T}{\sqrt{T}}\right),$$

where $T > 0$ us the total iteration number.

Adaptive Moment Estimation (ADAM), Kingma & Ba, 2017

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- ADAM is the combination of RMSProp and the gradient descent with momentum. Here is the ADAM update

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\text{(Momentum)}: \quad & m^{(k)} = \beta_1 m^{(k-1)} + (1-\beta_1)\boldsymbol{g}^{(k)} \\
\text{(RMSProp)}: \quad & \boldsymbol{G}^{(k)} = \beta_2 \boldsymbol{G}^{(k-1)} + (1-\beta_2)\boldsymbol{g}^{(k)}\boldsymbol{g}^{(k)^T} \\
\text{(Bias Correction)} \quad & \hat{m}^{(k)} = m^{(k)}/(1-\beta_1^k) \\
\text{(Bias Correction)} \quad & \hat{\boldsymbol{G}}^{(k)} = \boldsymbol{G}^{(k)}/(1-\beta_2^k) \\
\text{(Update)} \quad & \Theta^{(k+1)} = \Theta^{(k)} - \eta \mathrm{diag}(\hat{\boldsymbol{G}}^{(k)})^{-1/2}\hat{m}^{(k)}
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- Common choices of β_1 and β_2 are 0.9 and 0.99 resp. in practice.

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Numerical Experiment

- Linear regression
- Find local minimum

The experiments are conducted on Python 3.9.16, we developed our own algorithms instead of using an existing library/Package.

Numerical Experiment : Linear Regression

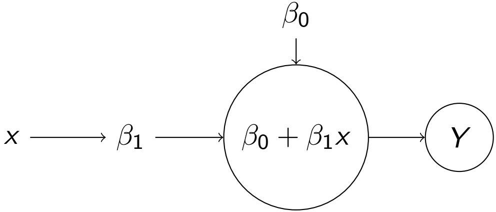
Given

$$
\begin{aligned}
& X \sim \mathcal{N}(0,1) \quad \varepsilon \sim \mathcal{N}(0,1) \\
& Y = \beta_0 + \beta_1 x + \varepsilon \\
& \text{Loss} = \frac{1}{n} \sum_{i=1}^{n} (Y_i - (\beta_0 + \beta_1 x_i))^2
\end{aligned}
$$

And the gradient of the loss function respect to β_0 and β_1 will be

$$
\begin{aligned}
\frac{\partial}{\partial \beta_0} \text{Loss} &= -\frac{2}{n} \sum_{i=1}^{n} Y_i - (\beta_0 + \beta_1 x_i) \\
\frac{\partial}{\partial \beta_1} \text{Loss} &= -\frac{2}{n} \sum_{i=1}^{n} Y_i - (\beta_0 + \beta_1 x_i) x_i
\end{aligned}
$$

We generate the (x_i, Y_i), for all $i \in [n]$ with $\beta_0 = 2$ and $\beta_1 = 3$.


β_0
x
β_1
$\beta_0 + \beta_1 x$
Y

$$
\begin{tikzcd}
 & & \beta_0 \arrow[d] & \\
x \arrow[r] & \beta_1 \arrow[r] & \beta_0 + \beta_1 x \arrow[r] & Y
\end{tikzcd}
$$

$\boxed{\text{Now we switch to PPT}}$.

Numerical Experiment : local/global minimum

Use function

$$z = f(x, y) = \frac{1}{2}x^2 + \frac{1}{4}y^4 - \frac{1}{2}y^2$$

Numerical Experiment : local/global minimum

Use function

$$z = f(x, y) = \frac{1}{2}x^2 + \frac{1}{4}y^4 - \frac{1}{2}y^2$$

By using "Second partial derivative test", critical points are $(0,0), (0,1), (0,-1)$ and local minimum at $(0,1)$ and $(0,-1)$, saddle point at $(0,0)$.

Numerical Experiment : local/global minimum

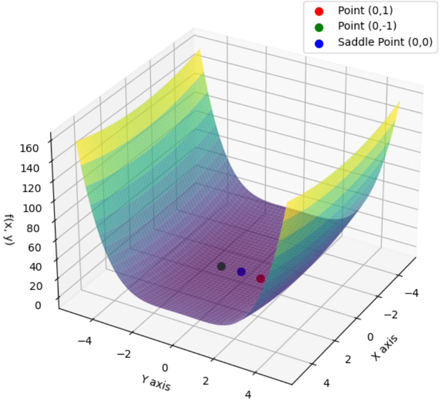
Use function

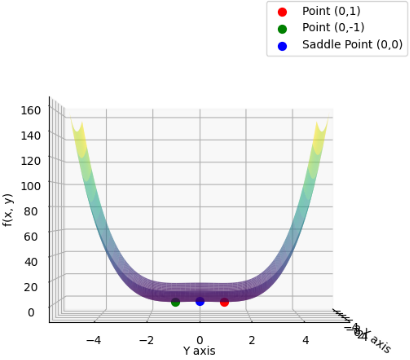
$$z = f(x, y) = \frac{1}{2}x^2 + \frac{1}{4}y^4 - \frac{1}{2}y^2$$

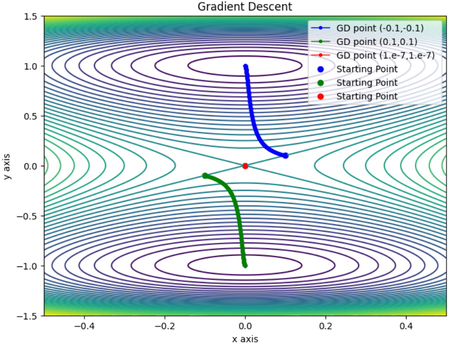
By using "Second partial derivative test", critical points are $(0,0), (0,1), (0,-1)$ and local minimum at $(0,1)$ and $(0,-1)$, saddle point at $(0,0)$. We will use the point nearby the saddle point as initial value such as $(0.1, 0.1)$, $(-0.1, -0.1)$ and $(10^{-7}, 10^{-7})$, and

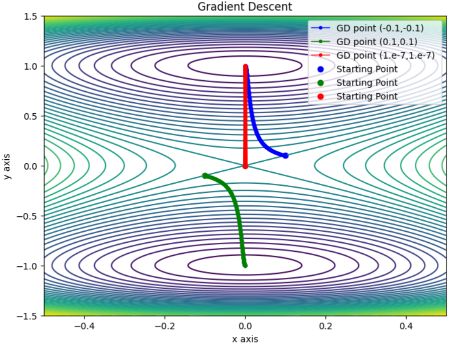
$$\nabla z = \begin{bmatrix} x \\ y^3 - y \end{bmatrix}$$

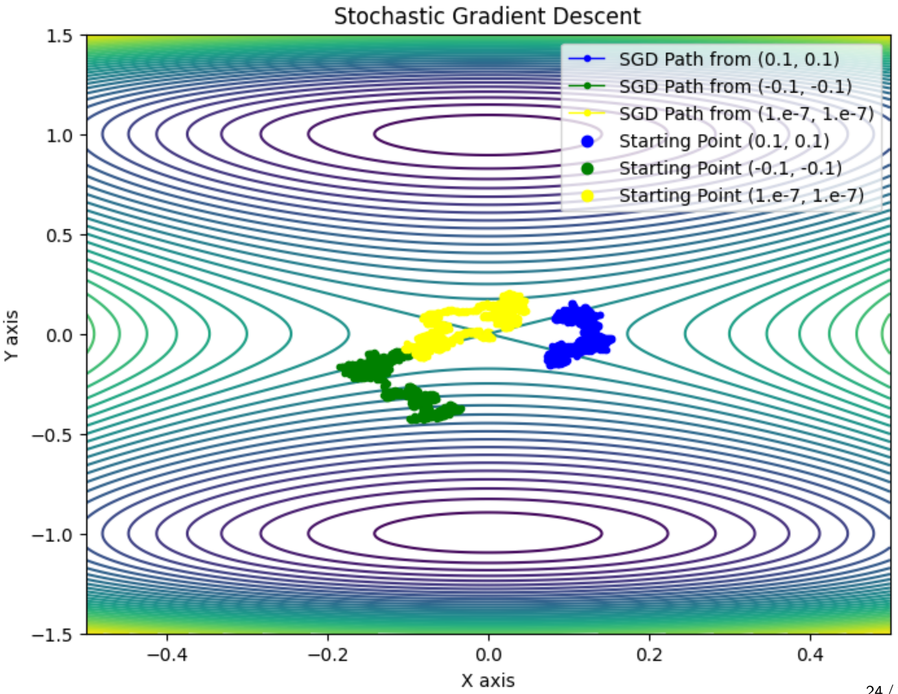
Function Overview

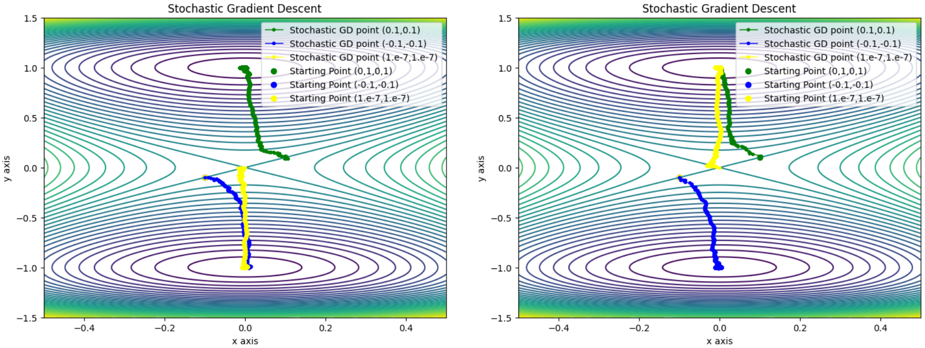


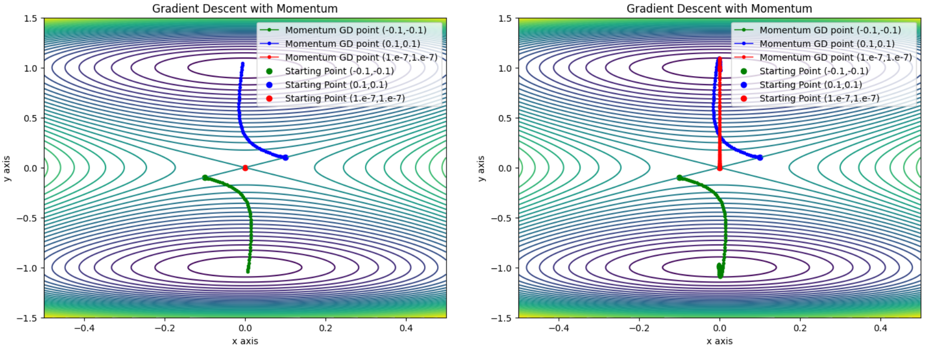


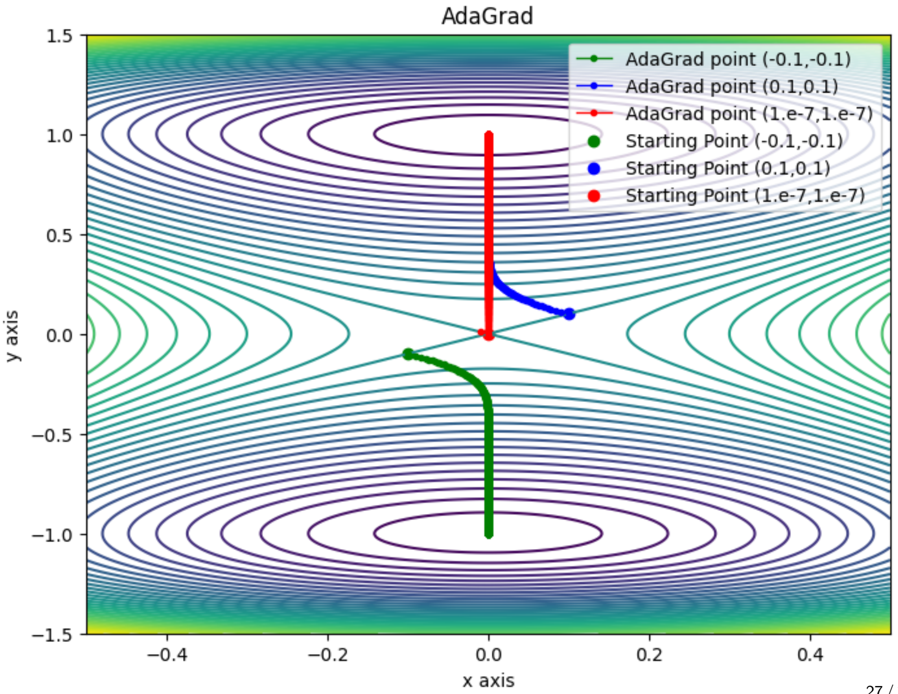

Gradient Descent
GD point (-0.1,-0.1)
GD point (0.1,0.1)
GD point (1.e-7,1.e-7)
Starting Point
Starting Point
Starting Point
y axis
x axis
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−0.4
−0.2
0.0
0.2
0.4


Gradient Descent
GD point (-0.1,-0.1)
GD point (0.1,0.1)
GD point (1.e-7,1.e-7)
Starting Point
Starting Point
Starting Point
y axis
x axis
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−0.4
−0.2
0.0
0.2
0.4

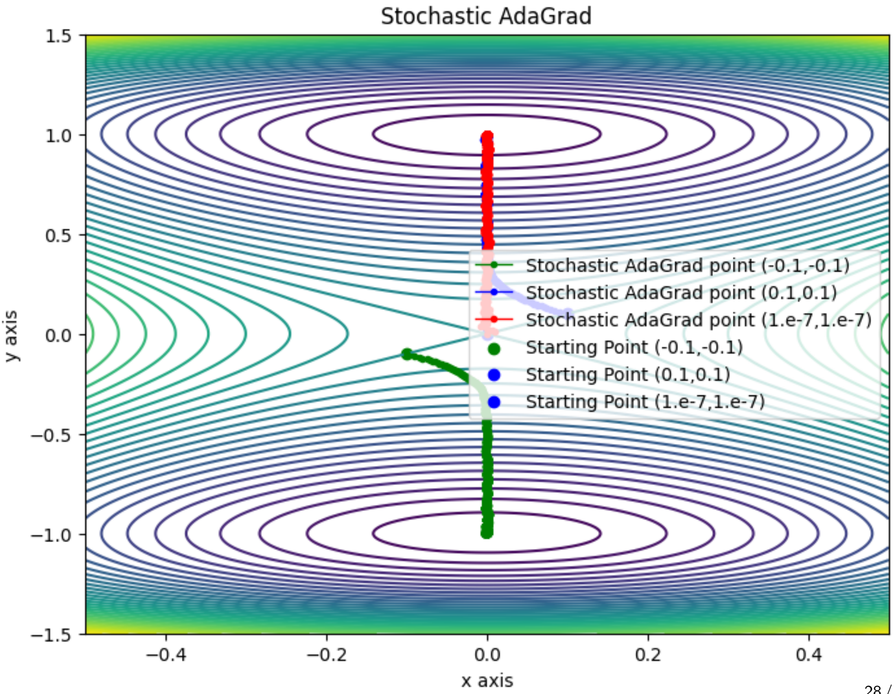

Stochastic Gradient Descent
SGD Path from (0.1, 0.1)
SGD Path from (-0.1, -0.1)
SGD Path from (1.e-7, 1.e-7)
Starting Point (0.1, 0.1)
Starting Point (-0.1, -0.1)
Starting Point (1.e-7, 1.e-7)
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−0.4
−0.2
0.0
0.2
0.4
Y axis
X axis

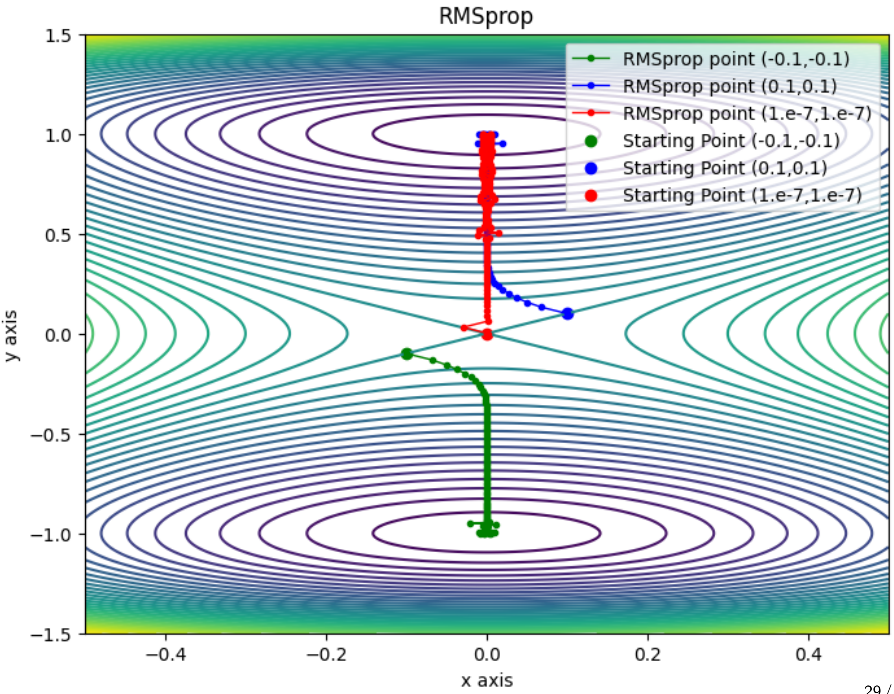

Stochastic Gradient Descent
Stochastic GD point (0.1,0.1)
Stochastic GD point (-0.1,-0.1)
Stochastic GD point (1.e-7,1.e-7)
Starting Point (0,1,0,1)
Starting Point (-0.1,-0.1)
Starting Point (1.e-7,1.e-7)
y axis
x axis
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−0.4
−0.2
0.0
0.2
0.4
Stochastic Gradient Descent
Stochastic GD point (0.1,0.1)
Stochastic GD point (-0.1,-0.1)
Stochastic GD point (1.e-7,1.e-7)
Starting Point (0,1,0,1)
Starting Point (-0.1,-0.1)
Starting Point (1.e-7,1.e-7)
y axis
x axis

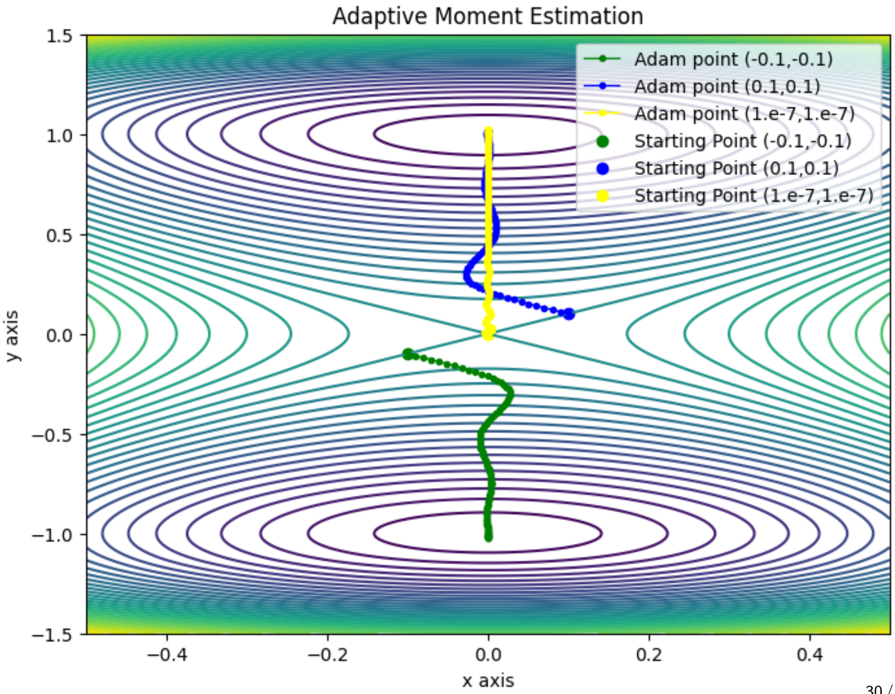

Gradient Descent with Momentum
Momentum GD point (-0.1,-0.1)
Momentum GD point (0.1,0.1)
Momentum GD point (1.e-7,1.e-7)
Starting Point (-0.1,-0.1)
Starting Point (0.1,0.1)
Starting Point (1.e-7,1.e-7)
x axis
y axis
Gradient Descent with Momentum
Momentum GD point (-0.1,-0.1)
Momentum GD point (0.1,0.1)
Momentum GD point (1.e-7,1.e-7)
Starting Point (-0.1,-0.1)
Starting Point (0.1,0.1)
Starting Point (1.e-7,1.e-7)
x axis
y axis



AdaGrad
AdaGrad point (-0.1,-0.1)
AdaGrad point (0.1,0.1)
AdaGrad point (1.e-7,1.e-7)
Starting Point (-0.1,-0.1)
Starting Point (0.1,0.1)
Starting Point (1.e-7,1.e-7)
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
y axis
−0.4
−0.2
0.0
0.2
0.4
x axis


Stochastic AdaGrad
Stochastic AdaGrad point (-0.1,-0.1)
Stochastic AdaGrad point (0.1,0.1)
Stochastic AdaGrad point (1.e-7,1.e-7)
Starting Point (-0.1,-0.1)
Starting Point (0.1,0.1)
Starting Point (1.e-7,1.e-7)
y axis
x axis
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−0.4
−0.2
0.0
0.2
0.4


RMSprop
RMSprop point (-0.1,-0.1)
RMSprop point (0.1,0.1)
RMSprop point (1.e-7,1.e-7)
Starting Point (-0.1,-0.1)
Starting Point (0.1,0.1)
Starting Point (1.e-7,1.e-7)
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−0.4
−0.2
0.0
0.2
0.4
x axis
y axis


Adaptive Moment Estimation
Adam point (-0.1,-0.1)
Adam point (0.1,0.1)
Adam point (1.e-7,1.e-7)
Starting Point (-0.1,-0.1)
Starting Point (0.1,0.1)
Starting Point (1.e-7,1.e-7)
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
y axis
−0.4
−0.2
0.0
0.2
0.4
x axis

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Thank you!