Optimization Algorithms in Machine Learning

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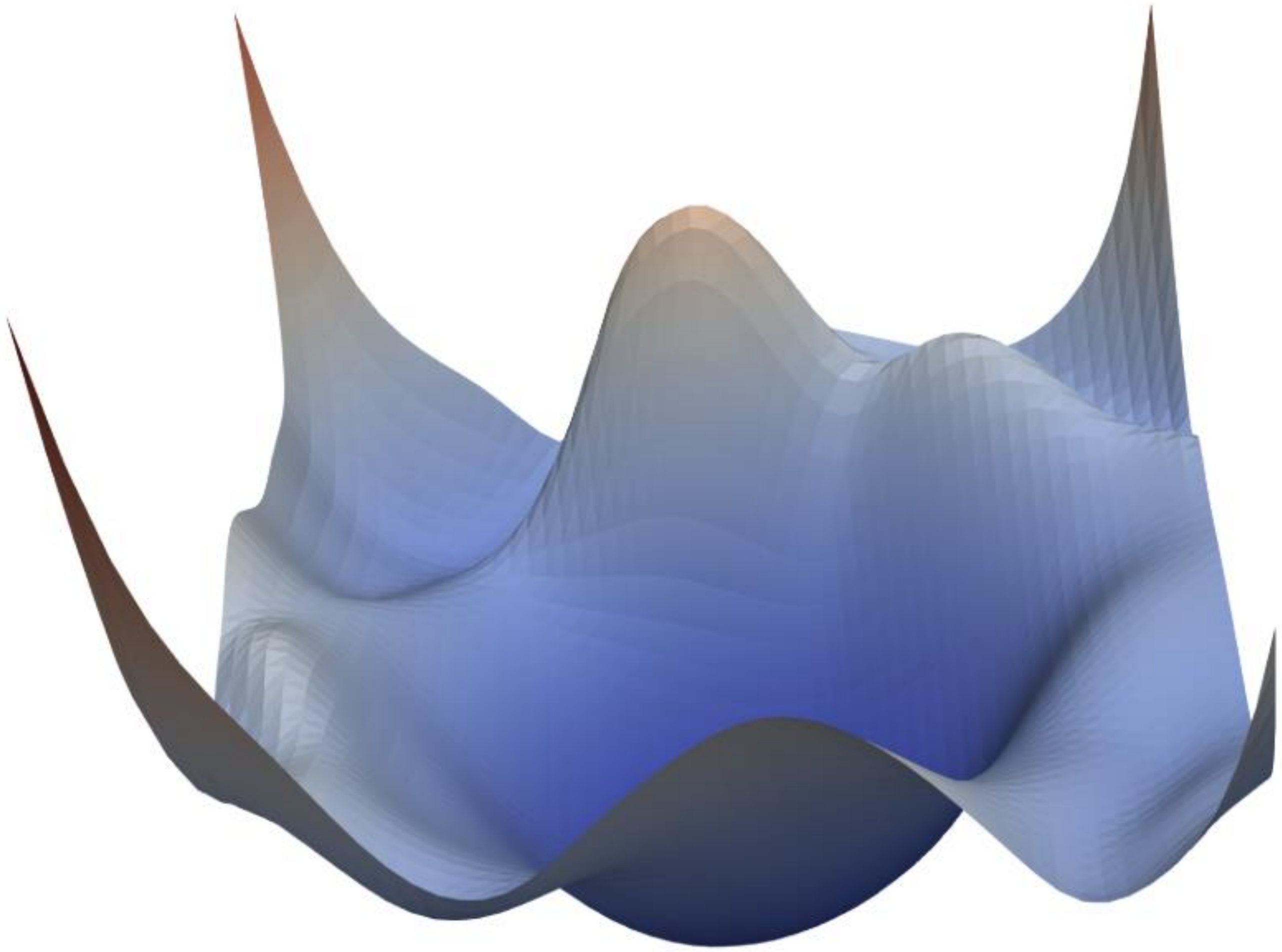
Recap: The General ML Problem

- Given training data $\{(x_1, y_1), \cdots, (x_N, y_N)\}$
- Assume Parameters are w (weights)
- General ML Optimization Problem:

$$\min_{w} \sum_{i=1}^{N} L(x_i, y_i, w) + \lambda R(w) \tag{1}$$

- $R(w)$ is a regularizer (either L1 or L2 regularization)

Most ML Problems are Non-Convex



Gradient Descent

- General ML Optimization Problem:

$$\min_{w} \sum_{i=1}^{N} L(x_i, y_i, w) + \lambda R(w) \tag{2}$$

- Gradient Descent computes the full gradient!
- Update equation: $w_{k+1} = w_k - \alpha_k \sum_{i=1}^{N} \nabla_w L(x_i, y_i, w) - \lambda \nabla_w R(w)$
- What is the problem with gradient descent?

Stochastic Gradient Descent

- Computing full gradient can be time consuming if N is very large!
- Idea of SGD: Compute an approximation of the full gradient and then move in that direction
- Idea: At iteration k, pick a random index i_k and then perform the following update:

$$w_{k+1} = w_k - \alpha_k \nabla f_{i_k}(w_k)$$

- Can be extended to minibatch setting as well.

SGD and Momentum

- Recall SGD:

$$w_{k+1} = w_k - \alpha_k \nabla f_{i_k}(w_k)$$

- Stochastic Momentum: Improves upon SGD via Momentum (similar to the GD case):

$$w_{k+1} = w_k - \alpha_k \nabla f_{i_k}(w_k + \gamma_t(w_k - w_{k-1})) + \beta_k(w_k - w_{k-1})$$

- Heavy Ball (HB) Momentum: $\gamma_k = 0$
- Nesterov's Accelerated Gradient (NAG): $\gamma_k = \beta_k$.

Another Variant of Momentum

- Another variant of Momentum used in Deep Learning is From the Gradient Accumulation Perspective
- Define Velocity v_t instead of the gradient

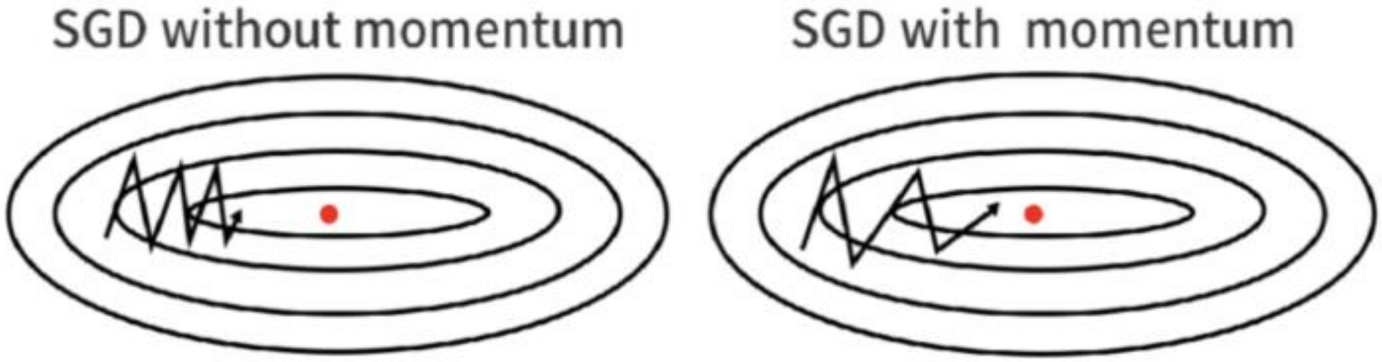
$$v_t = \gamma_t v_{t-1} + (1 - \gamma_t)\nabla L(\theta_t)$$

- In the above, γ_t is the momentum parameter, set to 0.9 for example
- Then we update the model parameters as:

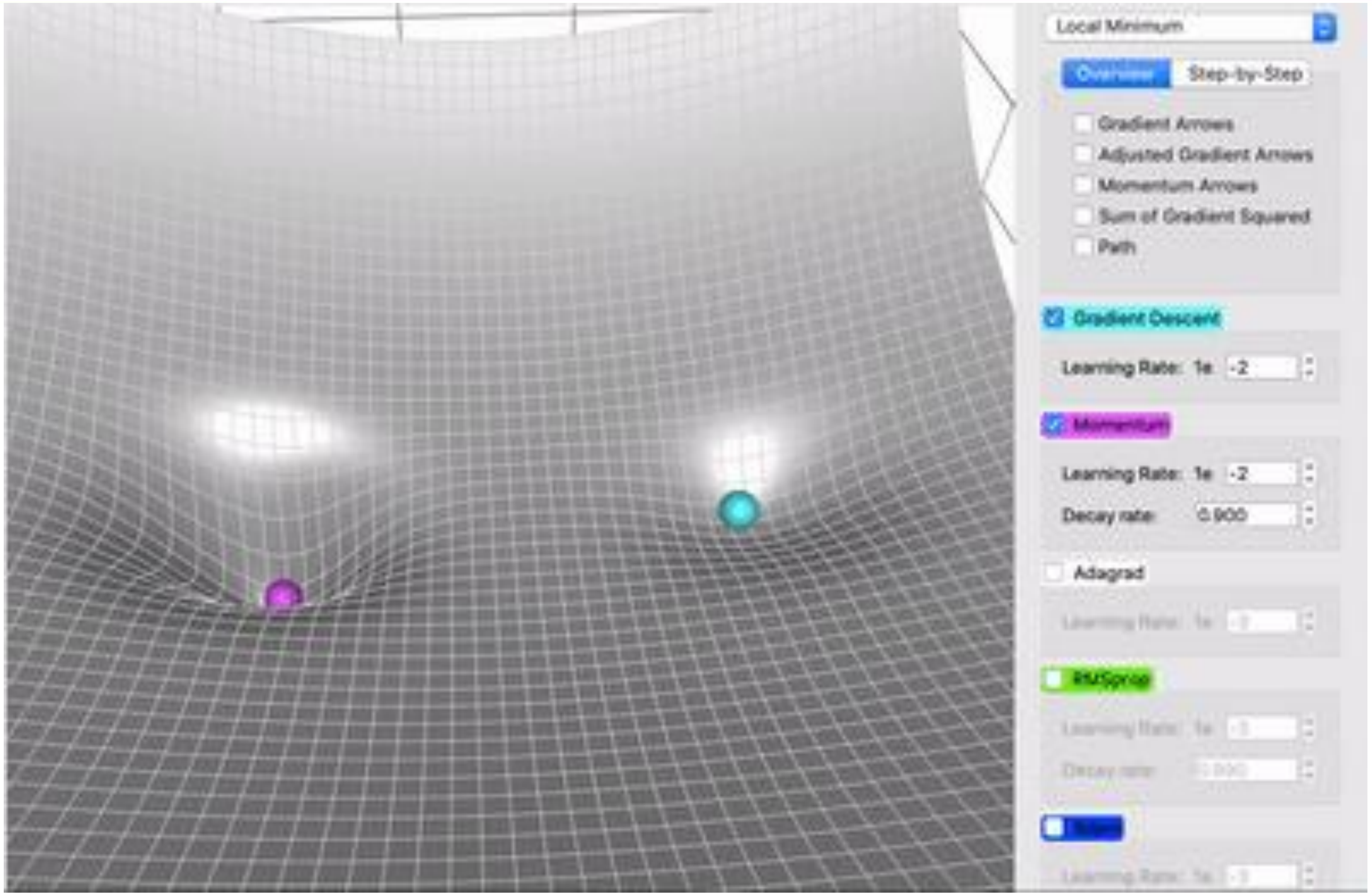
$$\theta_{t+1} = \theta_t - \eta_t \mathrm{v}_\mathrm{t}$$

Advantages of Momentum

- Avoid Local Minima: Momentum accelerates through small dips preventing the optimizer from getting stuck
- Reducing Oscillations: Momentum dampens oscillations especially in high-curvature areas
- Faster Convergence: By “remembering” past gradients, momentum accelerates convergence of the optimizers



SGD vs Momentum



✓ Gradient Descent
Learning Rate: 1e -2

✓ Momentum
Learning Rate: 1e -2
Decay rate: 0.900

Issue With SGD/Momentum

- These techniques are not adaptive: Require extensive tuning for learning rate schedules.
- Without the right LR schedule, convergence can be slow!
- They are also less robust to initialization
- Fix: Adapt learning rate based on gradient information until now.

Adaptive Gradient Descent Framework of Algorithms

- Adaptive Methods try to automatically adapt the learning rate.
- Define H_k as a positive semi-definite Matrix (recall the Hessian method?)
- The simplest Adaptive Algorithm called AdaGrad (Duchi et al 2011) is:

$$w_{k+1} = w_k - \alpha_k H_k^{-1} \nabla f_{i_k}(w_k)$$

  where H_k is a positive semi-definite Matrix!
- The simplest definition of H_k is a diagonal matrix (recall we need SGD algorithms to be super-fast, so no matrix inversion possible!)
- Define:

$$H_k = \text{diag}(\{\sum_{i=1}^{k} \eta_i g_i \circ g_i\}^{1/2})$$

AdaGrad Algorithm

1️⃣ Accumulate the Squares of Gradients

Adagrad keeps a **running sum of squares** of past gradients for each parameter:

$$G_t = G_{t-1} + g_t^2$$

- G_t is a vector (one value per parameter).
- g_t^2 means element-wise squaring.

2️⃣ Adapt the Learning Rate Per Parameter

The update rule becomes:

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

where:

- η = initial learning rate
- ϵ = small constant for numerical stability (like 10^{-8})
- $\odot$ = element-wise multiplication

AdaGrad Algorithm

🧩 Why Adagrad Helps:

- Great for **sparse data** (e.g., NLP, recommendation systems).
- Infrequent features get **larger steps** → faster learning.
- Frequent features slow down → prevent exploding updates.

🚨 Downside of Adagrad:

- G_t **keeps accumulating forever**.
- Eventually, learning rate becomes **too small** → training stalls.

✅ This is why later methods like **RMSProp** and **Adam** modify Adagrad by:

- Using a **moving average** instead of pure accumulation.

TLDR of AdaGrad

Basic Idea of AdaGrad:

- No need to worry about the learning rate
- SGD will diverge with a very large learning rate
- AdaGrad manages to adapt the learning rate so the initial learning rate is not a concern anymore!

Unified Framework of Adaptive Algorithms

- We can unify all adaptive and non-adaptive variants into a single update equation:

$$w_{k+1} = w_k - \alpha_k H_k^{-1} \nabla f_{i_k}(w_k + \gamma_k(w_k - w_{k-1})) + \beta_k H_k^{-1} H_{k-1}(w_k - w_{k-1})$$

- Recall $H_k = \mathrm{diag}(\{\sum_{i=1}^{k} \eta_i g_i \circ g_i\}^{1/2})$. Define $G_k = H_k \circ H_k$ and $D_k = \mathrm{diag}(g_k \circ g_k)$.

	SGD	HB	NAG	AdaGrad	RMSProp	Adam
G_k	I	I	I	$\mathrm{G}_{k-1} + \mathrm{D}_k$	$\beta_2 \mathrm{G}_{k-1} + (1-\beta_2)\mathrm{D}_k$	$\frac{\beta_2}{1-\beta_2^k}\mathrm{G}_{k-1} + \frac{(1-\beta_2)}{1-\beta_2^k}\mathrm{D}_k$
α_k	α	α	α	α	α	$\alpha\frac{1-\beta_1}{1-\beta_1^k}$
β_k	0	β	β	0	0	$\frac{\beta_1(1-\beta_1^{k-1})}{1-\beta_1^k}$
γ	0	0	β	0	0	0

More on ADAM

🧠 Motivation

- SGD struggles with noisy gradients and needs careful learning rate tuning.
- Adagrad shrinks learning rates too much over time.
- Momentum improves stability but still uses fixed learning rate.

✅ **Adam combines the best of Momentum + Adagrad.**

More on Adam

1️⃣ First Moment Estimate (Momentum)

Update the **running average of gradients**:

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

2️⃣ Second Moment Estimate

Update the **running average of squared gradients**:

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

3️⃣ Bias Correction

Correct initial bias in m_t and v_t:

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

4️⃣ Parameter Update

Update parameters using adapted step size:

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

Extensions

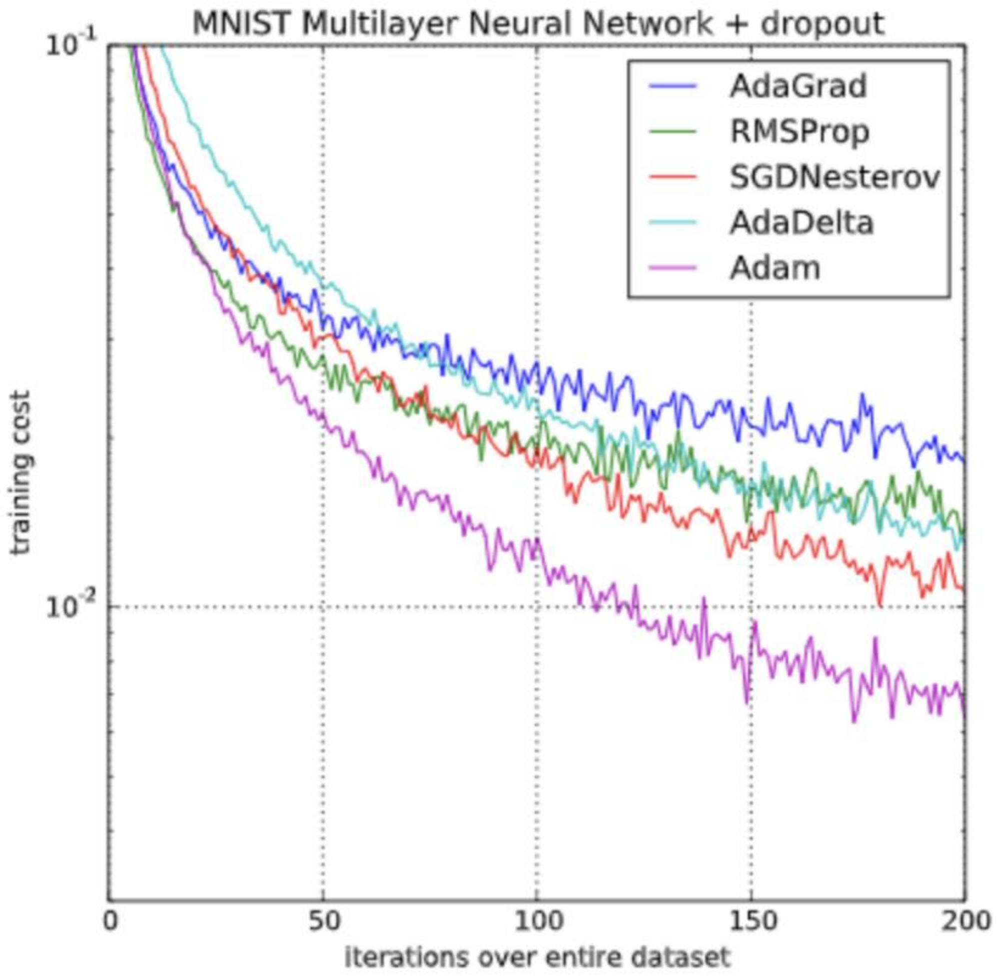
Numerous extensions of the above techniques

- AdaMax is an extension of ADAM to use the l_{infty} norm (i.e. max) instead of square.
- NADAM applies Nesterovs momentum instead of HB Momentum to Adaptive Methods.
- ADADelta is an extension of RMSProp to use the RMS operator on the weight differences as well.
- Recent Algorithm (AMSGrad) by Reddi et al (ICLR 2018) which fixes a theoretical error in ADAM (causing it to not converge even for convex functions) simply by ensuring v_t's remain positive!
- See more details to compare the different optimization algorithms (and also what they are) here: `https://ruder.io/optimizing-gradient-descent/`.

Comparison of Different Methods

- AdaGrad (Duchi et al 2011) is one of the most influential papers of the last decade!
- The starting point of numerous new techniques for adaptive methods.
- There is really no one technique that is provably better than the other. Each technique has its own pros and cons!
- In the next few slides, I'll try to put together a few takeaways from some recent papers which have studied this specifically for non-convex optimization.

ADAM Paper


MNIST Multilayer Neural Network + dropout
AdaGrad
RMSProp
SGDNesterov
AdaDelta
Adam
training cost
10^{-1}
10^{-2}
0
50
100
150
200
iterations over entire dataset

Adaptive vs Non Adaptive Techniques: Comparisons

- Benefits of AdaGrad: AdaGrad can significantly improve upon SGD in sparse feature sets! It automatically sets the learning rate, and secondly, automatically updates the learning rates with a decay schedule! Also, it has a per coordinate learning rate!
- In dense settings and particularly in deep models, Adagrad works very poorly because of rapid decay in learning rates
- ADAM, RMSProp, AdaDelta, ... all try to fix this issue!
- In many cases, these adaptive algorithms improve upon SGD in terms of training loss and better/faster convergence!
- Also, momentum generally improves upon the non-momentum variants!
- But....

SGD and Generalization

- But, in Machine Learning, Generalization is more important compared to just Training Loss!
- Recent works (for example, Wilson et al, The Marginal Value of Adaptive Gradient Methodsin Machine Learning) showed a very surprising result!
- Though adaptive gradient methods tend to minimize training loss better, they do so by obtaining more complex and less generalizable solutions!
- They gave a few synthetic examples (particularly in over0parameterized scenarios) where SGD and its variants obtain the less complex solutions but Adaptive variants obtain solutions which do not generalize well!

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