Optimization algorithms in deep learning

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Overview

What we'll cover today:

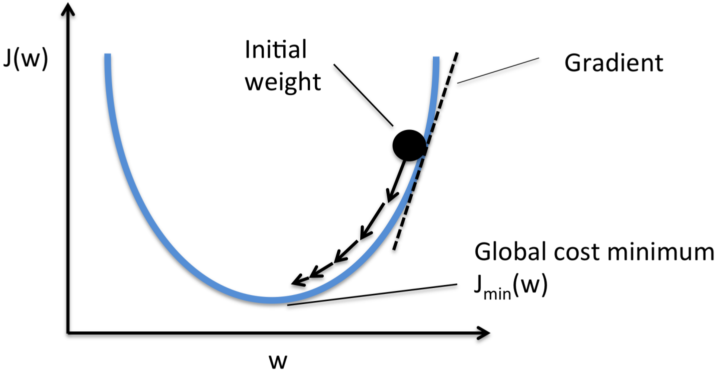
1. What is optimization?
2. Algorithms
   - SGD (Stochastic gradient descent)
   - SGD with Momentum
   - Adagrad (Adaptive learning rate)
3. Experiments
4. Summary
   - Discussion
   - Practicum

Optimization

In *context* of deep learning,
goal is to **minimize loss function**

$$w^* = \arg\min_{w} L(w) \tag{1}$$

What is gradient descent optimization?



Stochastic Gradient Descent (SGD)

Algorithm

Update step [1]:

$$\theta_{t+1} = \theta_t - \eta \cdot \nabla_\theta J(\theta_t) \tag{2}$$

where,

θ_t:	current model parameters
$\nabla_\theta J(\theta_t)$:	gradient of these model parameters
η:	learning rate (fixed)

Stochastic Gradient Descent (SGD)

How we usually call in PyTorch:

```
optimizer = optim.SGD(model.parameters(), lr=0.01)
```

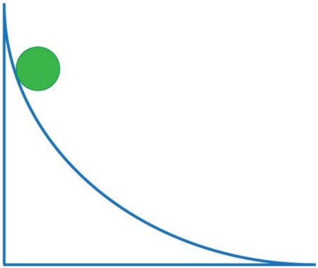
How we can create our "native" class [2]:

```
from torch.optim.optimizer import Optimizer

class CustomSGD(Optimizer):
  def __init__(self, model_params, lr=1e-3):
      self.model_params = list(model_params)
      self.lr = lr

  def zero_grad(self):
      for param in self.model_params:
          param.grad = None

  @torch.no_grad()
  def step(self):
      for param in self.model_params:
          param.sub_(self.lr * param.grad)
```

SGD with Momentum

General idea:

- Overcome small gradients near flat areas
- Build up from previous "velocity"
- Faster learning



SGD with Momentum

Algorithm

Update step [3]:

$$v_{t,i} = \gamma \cdot v_{t-1,i} + \nabla_\theta J(\theta_{t,i}) \tag{3}$$

$$\theta_{t+1} = \theta_t - \eta \cdot v_{t,i} \tag{4}$$

where,

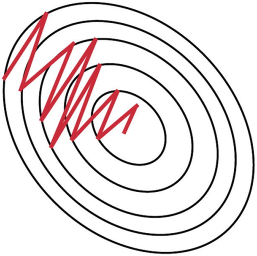
γ:	friction (or momentum, fixed)
v_t:	velocity
$\nabla_\theta J(\theta_t)$:	gradient of these model parameters
η:	learning rate (fixed)

SGD with Momentum

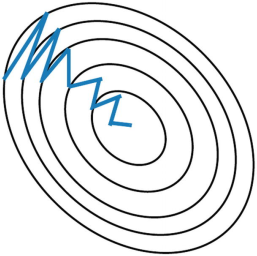
How we can create "native" `SGDMomentum` class:

```
from torch.optim.optimizer import Optimizer

class CustomSGDMomentum(Optimizer):
  def __init__(self, model_params, lr=1e-3, momentum=0.9):
      self.model_params = list(model_params)
      self.lr = lr
      self.momentum = momentum
      self.v = [torch.zeros_like(p) for p in self.model_params]

  def zero_grad(self):
      for param in self.model_params:
          param.grad = None

  @torch.no_grad()
  def step(self):
      for param, v in zip(self.model_params, self.v):
          v.mul_(self.momentum).add_(param.grad)
          param.sub_(self.lr * v)
```

SGD with Momentum



Stochastic Gradient Descent **withhout** Momentum



Stochastic Gradient Descent **with** Momentum

Adagrad

Algorithm

Update step [4]:

$$\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,i}} + \epsilon} \cdot \nabla_\theta J(\theta_{t,i}) \tag{5}$$

where,

$$G_{t,i} = G_{t-1,i} + (\nabla_\theta J(\theta_{t,i}))^2 \tag{6}$$

and,

$G_{t,i}$:	the sum of the squared gradients
ϵ:	a small number, to avoid division by zero
θ_t:	current model parameters
$\nabla_\theta J(\theta_t)$:	gradient of these model parameters
η:	learning rate (fixed)

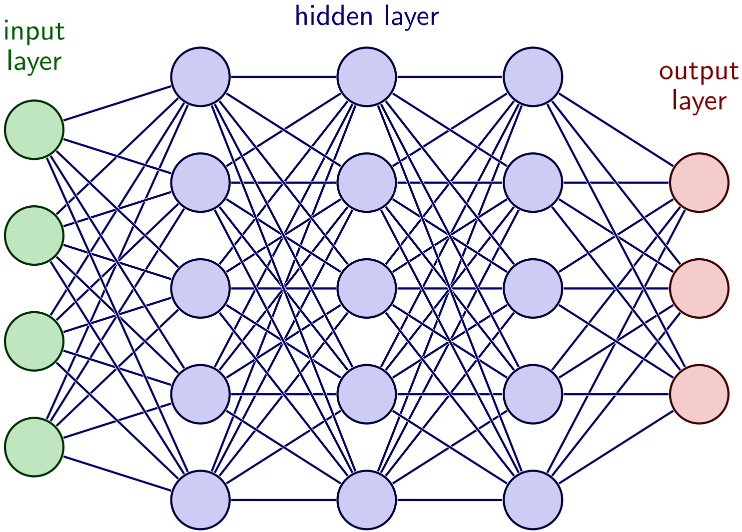
Adagrad

How we can create "native" `Adagrad` class:

```
from torch.optim.optimizer import Optimizer

class CustomAdagrad(Optimizer):
  def __init__(self, model_params, lr=1e-2, init_acc_sqr_grad=0, eps=1e-10)
      self.model_params = list(model_params)
      self.lr = lr
      self.acc_sqr_grads = [torch.full_like(p, init_acc_sqr_grad) for p in
      self.eps = eps

  def zero_grad(self):
      for param in self.model_params:
          param.grad = None

  @torch.no_grad()
  def step(self):
      for param, acc_sqr_grad in zip(self.model_params, self.acc_sqr_grads)
          acc_sqr_grad.add_(param.grad * param.grad)
          std = acc_sqr_grad.sqrt().add(self.eps)
          param.sub_((self.lr / std) * param.grad)
```

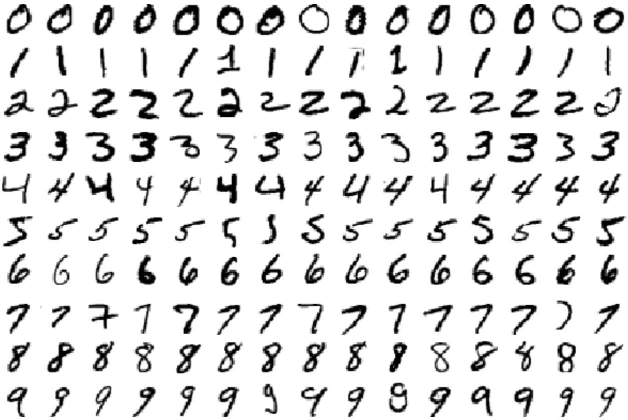
Experiment

A vanilla MLP (Multilayer Perceptron)



Experiment

MNIST dataset [5]



Experiment

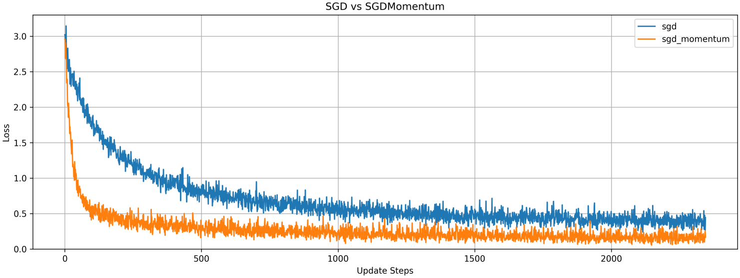


Figure 1: SGD vs momentum [git: CodeSeoul/machine-learning]

Experiment

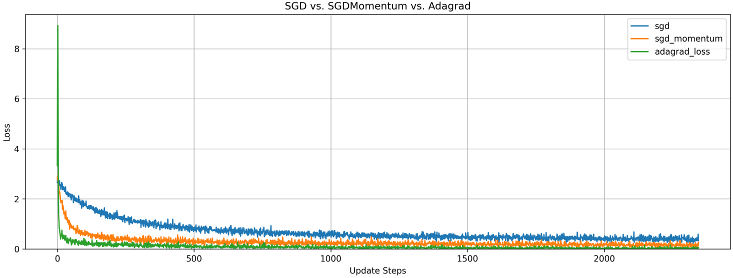


Figure 2: SGD vs momentum vs Adagrad [git: CodeSeoul/machine-learning]

Discussion

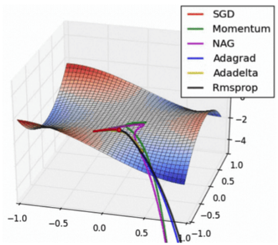


Figure 3: Trajectories of optimization algorithms in high-dimensional space [1]

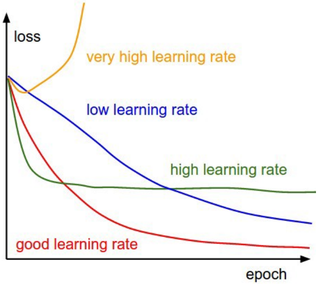


Figure 4: Selecting learning rate (lr) [6]

- The randomness introduced by SGD allows to reach better minimum. But in cases with many local minima, SGD may still get stuck.
- A systematic way to choose a good lr is by initially assigning it a very low value and increasing it slowly until the loss stops decreasing.

Practicum

Thank you for your attention!

- Workshop contents: https://github.com/CodeSeoul/machine-learning/tree/master/221105-optimization
- Follow-up QA? http://discord.com/users/tuttelikz

References

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