ADAPTIVE LEARNING RATE

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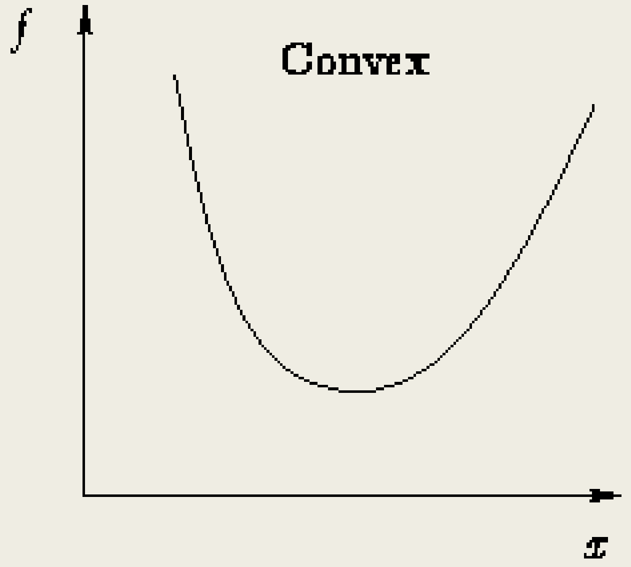
Motivation

- Basic methods have a fixed learning rate.

- Challenges of using learning rate scheduler
  - *Dependency of type of model and problem.*
  - *Same learning rate is applied on different parameters.*

- **Solution:** Adaptive learning rate.
- Adaptive learning rate is a method by which the performance of the model on the training dataset can be monitored by the learning algorithm and the learning rate can be adjusted in response.

AdaGrad



- The AdaGrad (**Ada**ptive **Grad**ient) algorithm, individually adapts the learning rates of all model parameters by scaling them inversely proportional to the square-root of the sum of all of their historical squared values.
- Adagrad uses a different learning rate for every parameter θ_i at every time step t.

- It has an improved performance over SGD.
- Mostly used in natural language processing and image recognition.

AdaGrad Algorithm

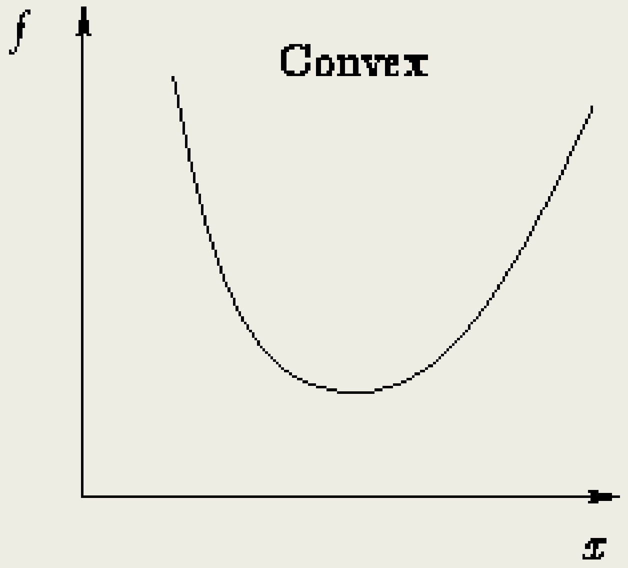
```
Require: Global learning rate
Require: Initial parameter
Require: small constant .(suggested value: $10^{-7}$)
  Initialize gradient accumulation variable $\boldsymbol{r} = \mathbf{0}$
  while stopping criterion not met do
     Sample a mini-batch of $m$ examples from the training set $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ with corresponding targets $y^{(i)}$.
     Compute gradient:
     Accumulate squared gradient:
     Compute update:
     Apply update
  end while
```

RMS Prop

- Problem with AdaGrad is its nature of radically diminishing learning rates and hence RMS Prop algorithm.
- RMSProp would deal with this problem and it is similar to gradient descent with momentum.

- RMSprop as well divides the learning rate by an exponentially decaying average of squared gradients.
- Usual values for is 0.9 or 0.95.
- RMSProp converges faster than AdaGrad to the convex bowl.
- It is useful when dealing with sparse data or noisy data.

RMSProp Algorithm



```
Require: Global learning rate , decay rate
Require: Initial parameter
Require: small constant .
  Initialize gradient accumulation variable r = 0
  while stopping criterion not met do
      Sample a mini-batch of m examples from the training set {$x^{(1)}$, $x^{(2)}$, …, $x^{(m)}$} with corresponding targets $y^{(i)}$.
      Compute gradient:
      Accumulate squared gradient:
      Compute update:
      Apply update
  end while
```

Adam

- The name is derived from the phrase "**Ada**ptive **m**oments".
- It estimates the first moment and the second moment of the gradients and hence the name of the method.
- It is a combines the advantages of AdaGrad and RMSProp.
  - *Inspired from AdaGrad, it maintains the per-parameter learning rate that improves performance of problems with sparse gradients.*
  - *Inspired from RMSProp, it stores the exponential decay of average of the past squared gradients.*

Adam Algorithm

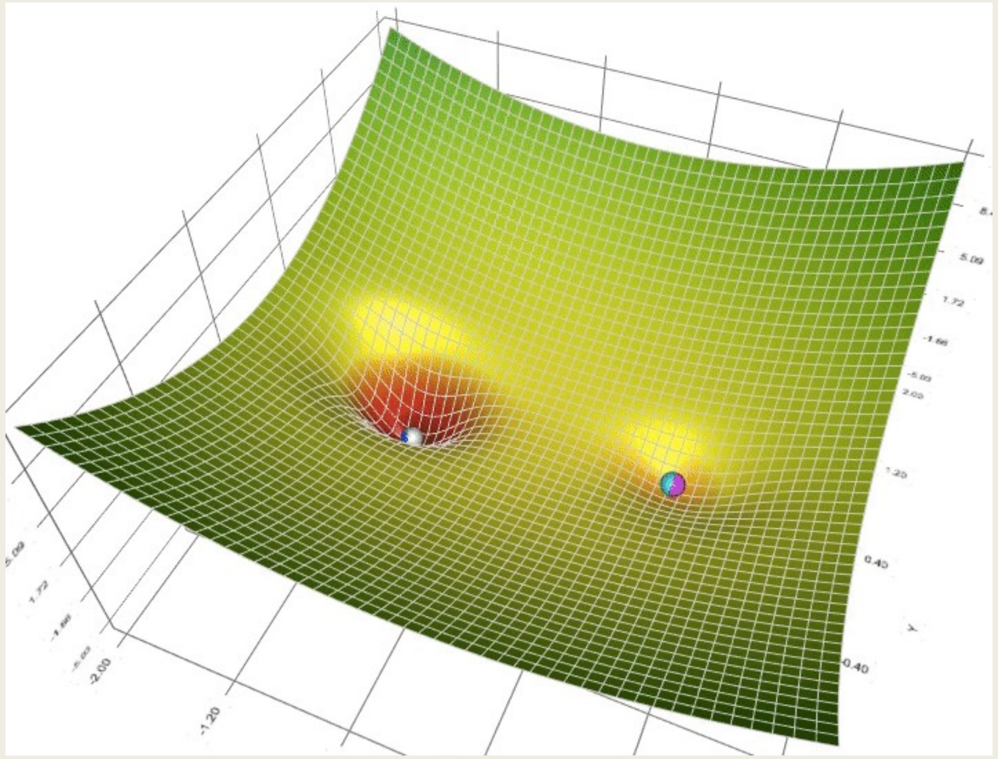
```
**Require:** step size  (suggested default: 0.001)
**Require:** Exponential decay rates for moment estimates, $\rho_1$ and $\rho_2$ in [0, 1).(Suggested defaults: 0.9 and 0.999 respectively)
**Require:** Small constant  used for numerical stabilization. (Suggested default: $10^{-8}$)
**Require:** Initial parameters .
  Initialize 1st and 2nd moment variables $s = 0$, $r = 0$
  Initialize time step $t = 0$
  **while** stopping criterion not met **do**
     Sample a mini-batch of $m$ examples from the training set $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ with corresponding targets $y^{(i)}$.
     Compute gradient:

     Update biased first moment estimate:
     Update biased second moment estimate:
     Correct bias in first moment:
     Correct bias in second moment:
     Compute update:
     Apply update:
  **end while**
```

Choosing the right optimization algorithm

- It is highly problem dependent.
- If the input data is highly sparse than adaptive learning rates are recommended.
- Adaptive models are used when training a deep or complex neural network or when faster convergence is expected.
- Adam is the mostly used optimizer.

Example

gradient descent (cyan), momentum (magenta), AdaGrad (white), RMSProp (green), Adam (blue).



Second-Order methods

- It provides an addition curvature information of an objective function that adaptively estimate the step-length of optimization trajectory in training phase of neural network.
- This involves computing or approximating the matrix of second-order derivatives, i.e. the Hessian, in the context of exact deterministic optimization.

$$\mathbf{H}f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n\,\partial x_1} & \frac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix},$$

- While second-order methods often have significantly better convergence properties than first-order methods, the size of typical problems prohibits their use in practice, as they require quadratic storage and cubic computation time for each gradient update.
- In all the methods here empirical risk is assumed to be

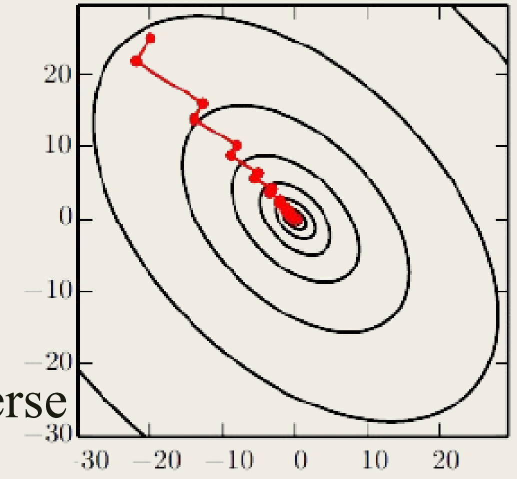
Newton’s Method

- It is a widely used second-order gradient method.
- It is a optimization method based on second order Taylor series expansion of J() at some point $_0$ after ignoring the higher orders.
- This method added computational burden of calculation of inverse of the matrix and also not recommended for a function with saddle points.
- For non-quadratic surfaces, as long as H remains PD, Newton’s method can be applied.
- Newton’s method would require the inversion of a $k \times k$ matrix—with computational complexity of $O(k^3)$.

Newton's method Algorithm

```
Require: Initial parameter
Require: Training set of $m$ examples
 while stopping criterion not met do
     Compute gradient:
     Compute Hessian:
     Compute Hessian inverse: $H^{-1}$
     Compute update: g
     Apply update
 end while
```

Conjugate gradients



- Conjugate gradients is a method to efficiently avoid the calculation of the inverse Hessian by iteratively descending conjugate directions.
- Motivation of this approach is line searches applied iteratively in the direction associated with the gradient.
- At each step, next step is made in the direction using
- Two directions are conjugate if
- Two methods of calculation are:

Fletcher-Reeves:

$$\beta_t = \frac{\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_t)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_t)}{\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_{t-1})^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_{t-1})}$$

Polak-Ribière:

$$\beta_t = \frac{(\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_t) - \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_{t-1}))^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_t)}{\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_{t-1})^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_{t-1})}$$

Conjugate gradient method

```
**Require**: Initial parameters $_0$
**Require:** Training set of $m$ examples
  Initialize
  Initialize $g_0 = 0$
  Initialize $t = 1$
  **while** stopping criterion not met **do**
     Initialize the gradient $g_t = 0$
     Compute gradient:
     Compute
     Compute search direction:
     Perform line search to find:
     Apply update:

  **end while**
```

Training Optimization II

Optimization Strategies and Meta-Algorithms

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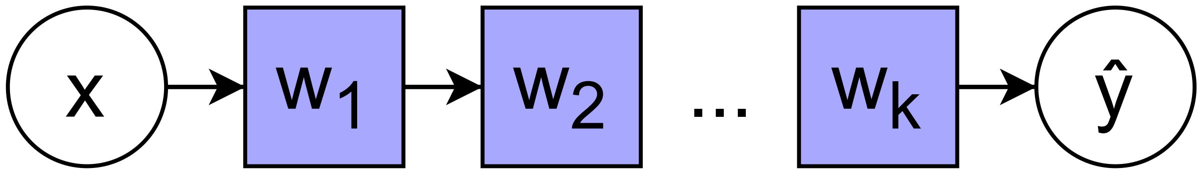
22.12.2020

Outline

Outline

Batch Normalization – Motivation



- $\hat{y} = x w_1 w_2 \cdots w_k$ (all $\in \mathbb{R}$)
- gradient of w_1 derived under the assumption that $w_2, \ldots, w_k$ fixed
- BUT: update rule $w \leftarrow w - \epsilon g$
- expected: $\hat{y}$ decreases by $\epsilon g^T g$ (first-order Taylor approximation)
- actually: various higher-order effects, e.g. $\epsilon^2 g_1 g_2 \prod_{i=3}^{k} w_i$

Batch Normalization

problem: unwanted side-effects when applying gradient-descent to networks with many layers

solutions

- correction via higher-order methods
- very small learning rate
- batch normalization

batch normalization:

- normalize activation values after each linear transformation
- applicable to all layers except for the output layer

Batch Normalization

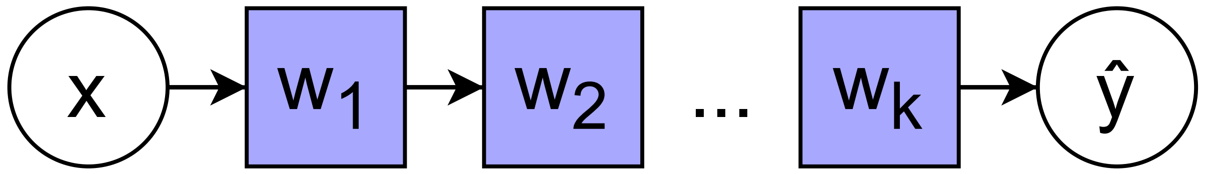
batch normalization

Input: m examples $e^{(i)} \in \mathbb{R}^n$ (n nodes in layer)

1. calculate n means $\mu_j = \frac{1}{m}\sum_{i=1}^m e_j^{(i)}$
2. calculate n standard deviations $\sigma_j = \sqrt{\delta + \frac{1}{m}\sum_{i=1}^m (e_j^{(i)} - \mu_j)^2}$ with a small positive δ (e.g. 10^{-8})
3. replace $e^{(i)}$ by $e'^{(i)} = (\frac{e_1^{(i)}-\mu_1}{\sigma_1}, \frac{e_2^{(i)}-\mu_2}{\sigma_2}, \dots, \frac{e_n^{(i)}-\mu_n}{\sigma_n})^T$

training: back-propagate through this normalization operation
$\Rightarrow$gradient will never propose changing mean or standard deviation
test: use averages over μ, σ collected during training

Batch Normalization – Example



- $\hat{y} = xw_1w_2 \cdots w_k$
- $x \sim \mathcal{N}(0, 1)$
- linear transformation: $xw_1 \sim \mathcal{N}(0, \sigma^2)$
- σ removed by batch normalization $\Rightarrow xw_1 \sim \mathcal{N}(0, 1)$

$\Rightarrow$ only w_k has an (linear) effect on the output value $\hat{y}$

Batch Normalization

batch normalization removes linear effects of hidden layers, but preserves non-linear effects.

advantages [2]

- learning becomes more stable
- higher learning rates possible
- models less sensitive to initialization values
- regularization effect, similar to Dropout in some cases

$\Rightarrow$ faster and better training results

Outline

Supervised Pretraining

sometimes training a model directly for a task is not possible

problems

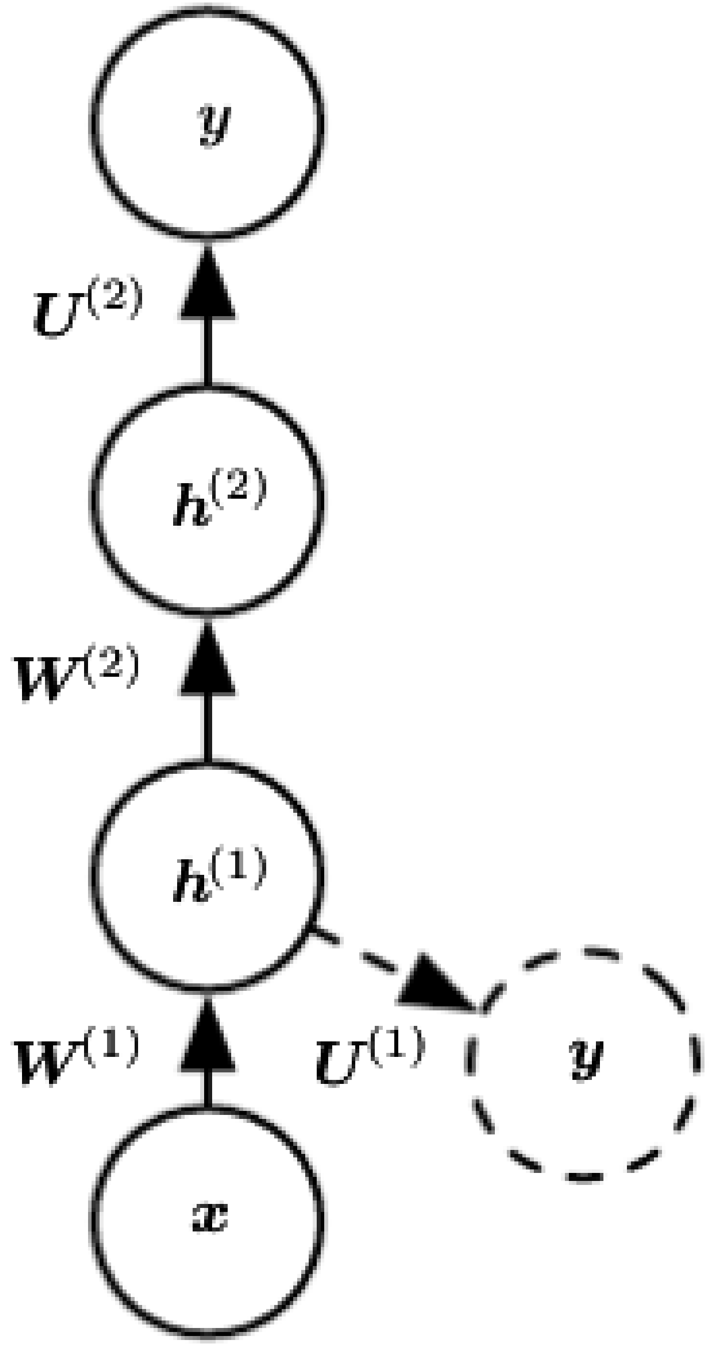
- hard to optimize model (e.g. very deep networks)
- difficult task

goal: additional guidance for parameters in deep networks

Supervised Pretraining

greedy supervised pretraining

- multiple trainings before actual training
- each trains only a subset of layers
- assumption: pre-trained weights provide guidance for hidden layer parameters



adapted from [1, p. 324]

Supervised Pretraining

teacher student learning

- shallow and wide network (teacher) aids training of deep and thin network (student)
- secondary objective: predict middle-layer values of teacher network
  $\Rightarrow$ guidance on how to use the hidden layers
- *example:* student outperforms teacher on CIFAR-10 with 90% less parameters [5]

Supervised Pretraining

transfer learning

- train network on one task
- use weights to initialize training on a similar task
- *assumption:* networks learn some general abstraction that is useful for many tasks

Outline

Designing Models to Aid Optimization

an easy to optimize model family is more important than a powerful optimization algorithm. [1, p. 326]

goal: local gradient information useful for reaching distant solution
$\Rightarrow$as much (near-)linearity as possible, e.g. ReLu instead of sigmoids

Designing Models to Aid Optimization

challenge: ensure useful gradient information on low layers in deep networks

skip connections [6]

- "highways" passing unchanged activation over several layers

auxiliary heads [7, 3]

- additional nodes at hidden layers
- trained to perform like output nodes, discarded after training

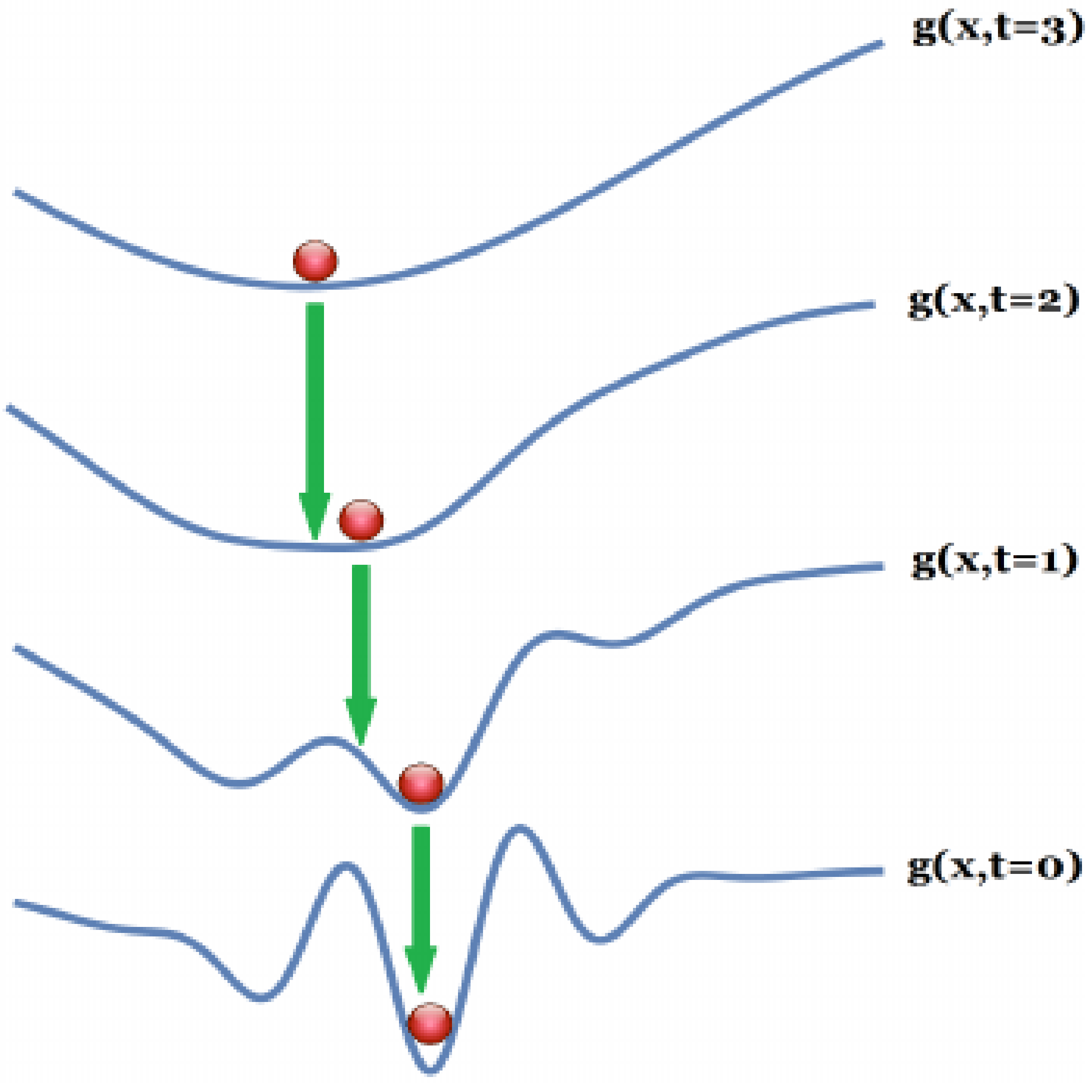
Outline

Continuation Methods

- generate series of cost functions $J^{(0)}, J^{(1)}, \ldots, J^{(n)} = J$ with increasing difficulty

$\Rightarrow$ keep local optimization in well-behaved regions

- often created by smoothing/blurring J
- intuition: non-convex function might become convex, but still preserve global minima



from [4]

Curriculum Learning

- first learn simple concept, then proceed to more complicated ones
- interpretation: series of $J^{(i)}$; cost functions with lower index depend on simpler examples
- successful in natural language processing and computer vision

Outline

Coordinate Descent

concept: only update a subset of parameters at each optimization step

example: k-means

objective function:

$$J(\mu_1, \ldots, \mu_k, S_1, \ldots, S_k) = \sum_{i=1}^{k} \sum_{x_j \in S_i} \|x_j - \mu_i\|^2 \ (S_i \text{ partition})$$

Lloyd's algorithm:

1. Select k random cluster centers
2. repeat until convergence
    1. assign each instance to closest center $\Rightarrow$ optimize w.r.t. S_i
    2. compute centers of this new clusters $\Rightarrow$ optimize w.r.t. μ_i

limitation: not applicable with strong dependencies between variables.

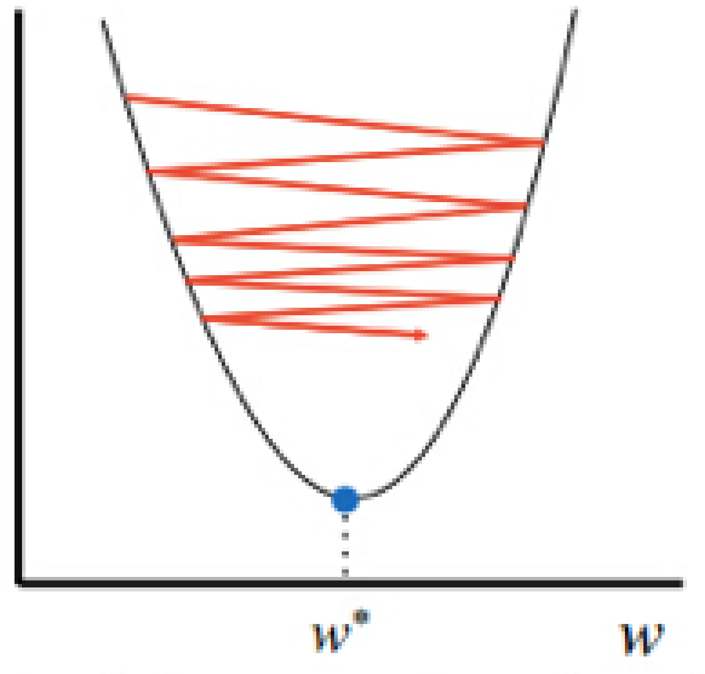
Polyak Averaging

- average over all locations visited by an optimization algorithm

$$\hat{\theta}^{(t)} = \frac{1}{t}\sum_{i=1}^{t}\theta^{(i)}$$

$\Rightarrow$ strong convergence guarantees for some problem classes

- for neural networks: no guarantees, but performs well in practice
- common modification: exponentially decaying running average



adapted from [8]

Outline

References I

[1] Ian Goodfellow et al. *Deep learning*. Vol. 1. 2. MIT press Cambridge, 2016.

[2] Sergey Ioffe and Christian Szegedy. "Batch normalization: Accelerating deep network training by reducing internal covariate shift". In: *arXiv preprint arXiv:1502.03167* (2015).

[3] Chen-Yu Lee et al. "Deeply-supervised nets". In: *Artificial intelligence and statistics*. 2015, pp. 562–570.

[4] Hossein Mobahi and John W Fisher III. "A theoretical analysis of optimization by gaussian continuation.". In: *AAAI*. Vol. 3. Citeseer. 2015, p. 3.

[5] Adriana Romero et al. "Fitnets: Hints for thin deep nets". In: *arXiv preprint arXiv:1412.6550* (2014).

References II

[6] Rupesh Kumar Srivastava, Klaus Greff, and Jürgen Schmidhuber. "Highway networks". In: *arXiv preprint arXiv:1505.00387* (2015).

[7] Christian Szegedy et al. "Going deeper with convolutions". In: *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2015, pp. 1–9.

[8] Varma and Das. *Deep Learning*. [accessed 2020-12-19]. 2018. URL: `https://srdas.github.io/DLBook`.

[9] Haohan Wang and Bhiksha Raj. "A survey: Time travel in deep learning space: An introduction to deep learning models and how deep learning models evolved from the initial ideas". In: (Oct. 2015).

Whiteboard