Machine Learning

Lecture 6: Optimization

Prof. Dr. Stephan Günnemann

Data Analytics and Machine Learning
Technical University of Munich

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Motivation

- Many machine learning tasks are optimization problems
- Examples we've already seen:
  - Linear Regression $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \frac{1}{2}(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^T(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$ LS
  - Logistic Regression $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} -\ln p(\boldsymbol{y} \mid \boldsymbol{w}, \boldsymbol{X})$ negative log
- Other examples:
  - Support Vector Machines: find hyperplane that separates the classes with a maximum margin
  - k-means: find clusters and centroids such that the squared distances is minimized
  - Matrix Factorization: find matrices that minimize the reconstruction error
  - Neural networks: find weights such that the loss is minimized
  - And many more...

General Task

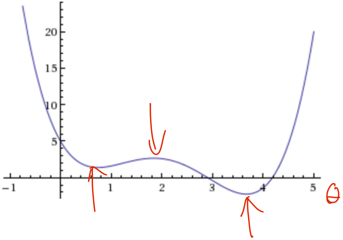
- Let $\boldsymbol{\theta}$ denote the variables/parameters of our problem we want to learn
  - e.g. $\boldsymbol{\theta} = \boldsymbol{w}$ in Logistic Regression
- Let $\mathcal{X}$ denote the domain of $\boldsymbol{\theta}$; the set of valid instantiations
  - constraints on the parameters!
  - e.g. $\mathcal{X}$ = set of (positive) real numbers
- Let $f(\boldsymbol{\theta})$ denote the objective function
  - e.g. f is the negative log likelihood
- Goal: Find solution $\boldsymbol{\theta}^*$ minimizing function $f : \boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta} \in \mathcal{X}} f(\boldsymbol{\theta})$
  - find a global minimum of the function f!
  - similarly, for some problems we are interested in finding the maximum

Introductory Example

- Goal: Find minimum of function
  $f(\theta) = 0.6 * \theta^4 - 5 * \theta^3 + 13 * \theta^2 - 12 * \theta + 5$

- Unconstrained optimization + differentiable function

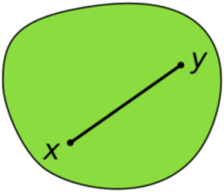
- Necessary condition for minima
  - Gradient = 0
  - Sufficient?

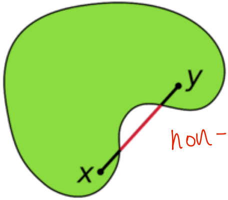


- General challenge: multiple local minima possible

Convexity: Sets

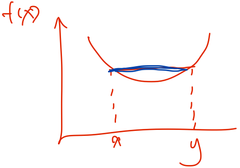
- X is a convex set
  iff
  for all $x, y \in X$ it follows that $\lambda x + (1 - \lambda)y \in X$ for $\lambda \in [0, 1]$



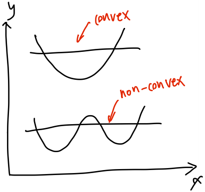


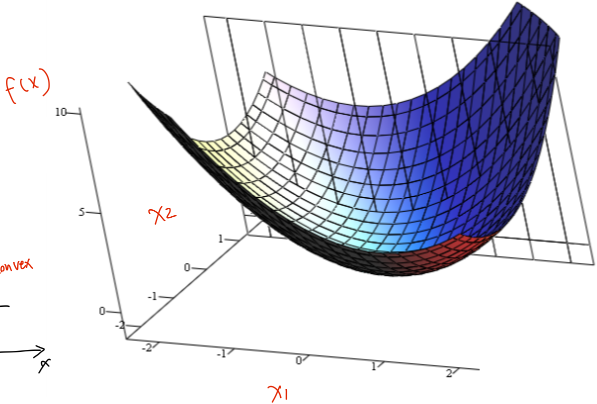
non-convex

Convexity: Functions



- $f(\boldsymbol{x})$ is a convex function on the convex set X
  iff
  for all $\boldsymbol{x}, \boldsymbol{y} \in X : \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y}) \geq f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y})$ for $\lambda \in [0,1]$



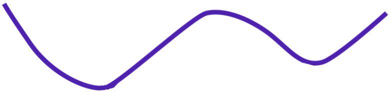


Convexity and *minimization problems*

- Region above a convex function is convex

$$f(\lambda \boldsymbol{x} + (1-\lambda)\boldsymbol{y}) \leq \lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y})$$
hence $\lambda f(\boldsymbol{x}) + (1-\lambda) f(\boldsymbol{y}) \in X$ for $\boldsymbol{x}, \boldsymbol{y} \in X$

- Convex functions have no local minima which are not global minima
  - Proof by contradiction - linear interpolation breaks local minimum condition



- Each local minimum is a global minimum
  - zero gradient implies (local) minimum for convex functions
  - if f_0 is a convex function and $\nabla f_0(\boldsymbol{\theta}^*) = 0$ then $\boldsymbol{\theta}$ is a gobal minimum
  - minimization becomes "relatively easy"

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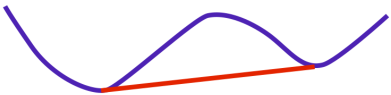

multiple global minimum

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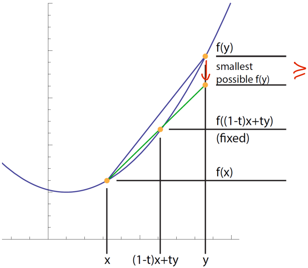
First order convexity conditions (I)

- Convexity imposes a rate of rise on the function

- $f((1-t)\boldsymbol{x}+t\boldsymbol{y}) \leq (1-t)f(\boldsymbol{x})+tf(\boldsymbol{y})$
- $f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq \frac{f((1-t)\boldsymbol{x}+t\boldsymbol{y})-f(\boldsymbol{x})}{t}$



- Difference between $f(\boldsymbol{y})$ and $f(\boldsymbol{x})$ is bounded by function values between $\boldsymbol{x}$ and $\boldsymbol{y}$

First order convexity conditions (II)

$$\underbrace{\left[f(x+\overset{\to 0}{\boxed{t(y-x)}}) - f(x) \right]}_{\boxed{t\,(y-x)} \to 0}(y-x)$$

- $f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq \frac{f((1-t)\boldsymbol{x}+t\boldsymbol{y})-f(\boldsymbol{x})}{t}$
- Let $t \to 0$ and apply the definition of the derivative
- $f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq (\boldsymbol{y}-\boldsymbol{x})^T \nabla f(\boldsymbol{x})$

$$\underbrace{\left[\frac{f(x+\xi)-f(x)}{\xi}\right]}_{\xi \to 0 \quad \nabla f(x)}(y-x)$$

- Theorem:

  Suppose $f : X \to \mathbb{R}$ is a differentiable function and X is convex. Then f is convex iff for $\boldsymbol{x}, \boldsymbol{y} \in X$

$$f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + (\boldsymbol{y}-\boldsymbol{x})^T \nabla f(\boldsymbol{x})$$

- Proof. See Boyd p.70

Verifying convexity (I)

- Convexity makes optimization "easier"
- How to verify whether a function is convex?

- For example: $e^{x_1+2*x_2} + x_1 - \log(x_2)$ convex on $[1, \infty) \times [1, \infty)$?

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1. Prove whether the definition of convexity holds (See slide 6)

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2. Exploit special results

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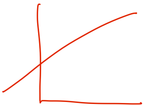
- How to verify whether a function is convex?

- For example: $e^{x_1+2*x_2} + x_1 - \log(x_2)$ convex on $[1, \infty) \times [1, \infty)$?

1. Prove whether the definition of convexity holds (See slide 6)
2. Exploit special results
   - First order convexity (See slide 9)
   - Example: A twice differentiable function of one variable is convex on an interval if and only if its second-derivative is non-negative on this interval
   - More general: a twice differentiable function of several variables is convex (on a convex set) if and only if its Hessian matrix is positive semidefinite (on the set)

Verifying convexity (II)



$\cup$ convex

$\cap$ concave

3. Show that the function can be obtained from simple convex functions by operations that preserve convexity

a) Start with simple convex functions, e.g.

- $f(x) = \text{const}$ and $f(\boldsymbol{x}) = \boldsymbol{x}^T \cdot \boldsymbol{b}$ (there are also concave functions)
- $f(x) = e^x$

b) Apply "construction rules" (next slide)

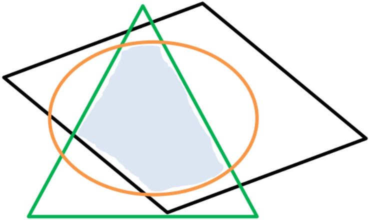
Convexity preserving operations

- Let $f_1 : \mathbb{R}^d \to \mathbb{R}$ and $f_2 : \mathbb{R}^d \to \mathbb{R}$ be convex functions, and $g : \mathbb{R}^d \to \mathbb{R}$ be a concave function, then
  - $h(\boldsymbol{x}) = f_1(\boldsymbol{x}) + f_2(\boldsymbol{x})$ is convex
  - $h(\boldsymbol{x}) = \max\{f_1(\boldsymbol{x}), f_2(\boldsymbol{x})\}$ is convex
  - $h(\boldsymbol{x}) = c \cdot f_1(\boldsymbol{x})$ is convex if $c \geq 0$
  - $h(\boldsymbol{x}) = c \cdot g(\boldsymbol{x})$ is convex if $c \leq 0$
  - $h(\boldsymbol{x}) = f_1(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$ is convex ($\boldsymbol{A}$ matrix, $\boldsymbol{b}$ vector)
  - $h(\boldsymbol{x}) = m(f_1(\boldsymbol{x}))$ is convex if $m : \mathbb{R} \to \mathbb{R}$ is convex and nondecreasing

- Example: $\underbrace{e^{x_1+2*x_2} + x_1}_{\text{convex}} \underbrace{- \log(x_2)}_{\substack{\text{convex} \\ (-1)\cdot\text{concave}}}$ is convex on, e.g., $[1, \infty) \times [1, \infty)$

Verifying convexity of sets

1. Prove definition
   – often easier for sets than for functions
2. Apply intersection rule
   – Let A and B be convex sets, then $A \cap B$ is a convex set



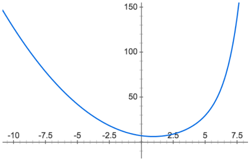
An easy problem

Convex objective function f

- Objective function differentiable on its whole domain
  - i.e. we are able to compute gradient f' at every point
- We can solve $f'(\boldsymbol{\theta}) = 0$ for $\boldsymbol{\theta}$ analytically
  - i.e. solution for $\boldsymbol{\theta}$ where gradient $= 0$ is known
- Unconstrained minimization
  - i.e. above computed solution for $\boldsymbol{\theta}$ is valid
- We are done!

- Example: Ordinary Least Squares Regression

$$x^2 + e^{x-3} - 2x + 7$$

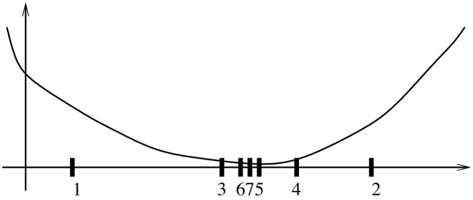


Outlook

- Unfortunately, many problems are harder...
- No analytical solution for $f'(\boldsymbol{\theta}) = 0$
  - e.g. Logistic Regression
  - Solution: try numerical approaches, e.g. gradient descent
- Constraint on $\boldsymbol{\theta}$
  - e.g. $f'(\boldsymbol{\theta}) = 0$ only holds for points outside the domain
  - Solution: constrained optimization
- f not differentiable on the whole domain
  - Potential solution: subgradients; or is it a discrete optimization problem?
- f not convex
  - Potential solution: convex relaxations; convex in some variables?

One-dimensional problems

- Key Idea
  - For differentiable f search for θ with $\nabla f(\theta) = 0$
  - Interval bisection (derivative is monotonic)



Require: $a, b,$ Precision ϵ

    Set $A = a, B = b$

    repeat

        if $f'(\frac{A+B}{2}) > 0$ **then**

            $B = \frac{A+B}{2}$

solution on the left

        else

            $A = \frac{A+B}{2}$

        end if

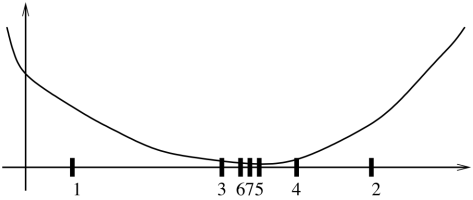
    until

    $(B - A)\min(|f'(A)|, |f'(B)|) \leq \epsilon$

Output: $x = \frac{A+B}{2}$

One-dimensional problems

- Key Idea
  - For differentiable f search for θ with $\nabla f(\theta) = 0$
  - Interval bisection (derivative is monotonic)
- Can be extended to nondifferentiable problems



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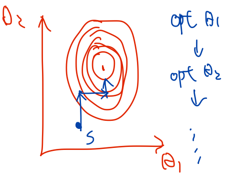
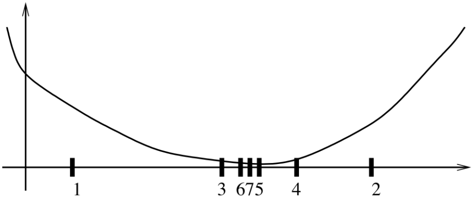
One-dimensional problems

coordinate descent



- Key Idea
  - For differentiable f search for θ with $\nabla f(\theta) = 0$
  - Interval bisection (derivative is monotonic)
- Can be extended to nondifferentiable problems
  - exploit convexity in upper bound and keep 5 points



Require: $a, b,$ Precision ϵ
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until
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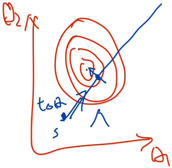
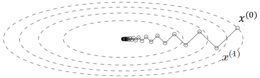
Output: $x = \frac{A+B}{2}$

solution on the left

Gradient Descent



- Key Idea
  - Gradient points into steepest ascent direction
  - Locally, the gradient is a good approximation of the objective function

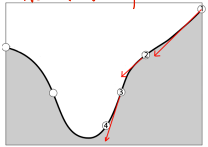


- GD with Line Search
  - Get descent direction, then unconstrained line search
  - Turn a multidimensional problem into a one-dimensional problem that we already know how to solve

given a starting point $\boldsymbol{\theta} \in \mathrm{Dom}(f)$
repeat
1. $\Delta\boldsymbol{\theta} := -\nabla f(\boldsymbol{\theta})$
2. Line search. $t^* = \arg\min_{t>0} f(\boldsymbol{\theta} + t \cdot \Delta\boldsymbol{\theta})$
3. Update. $\boldsymbol{\theta} := \boldsymbol{\theta} + t^* \Delta\boldsymbol{\theta}$

until stopping criterion is satisfied.

non-convex problem



Gradient Descent convergence

- Let p^* be the optimal value, $\boldsymbol{\theta}^*$ be the minimizer - the point where the minimum is obtained, and $\boldsymbol{\theta}^{(0)}$ be the starting point

- For strongly convex f (replace $\geq$ with $>$ in the definition of convexity) the residual error ρ, for the k-th iteration is:

$$\rho = f(\boldsymbol{\theta}^{(k)}) - p^* \leq c^k (f(\boldsymbol{\theta}^{(0)}) - p^*), \quad c < 1$$

$f(\boldsymbol{\theta}^{(k)})$ converges to p^* as $k \to \infty$

- We must have $f(\boldsymbol{\theta}^{(k)}) - p^* \leq \epsilon$ after at most $\frac{\log((f(\boldsymbol{\theta}^{(0)}) - p^*)\epsilon)/}{\log(1/c)}$ iterations

fast converge

0.01

0.001

- Linear convergence for strongly convex objective
  - $k \sim \log(\rho^{-1}) \qquad // \ k =$ number of iterations, ρ

- Linear convergence for strongly convex objective
  - i.e. linear when plotting on a log scale - old statistics terminology

Distributed/Parallel implementation

- Often problems are of the form
  - $f(\boldsymbol{\theta}) = \sum_i L_i(\boldsymbol{\theta}) + g(\boldsymbol{\theta})$
  - where i iterates over, e.g., each data instance
- Example OLS regression: // with regularization
  - $L_i(\boldsymbol{w}) = (\boldsymbol{x}_i^T \boldsymbol{w} - y_i)^2$ $g(\boldsymbol{w}) = \lambda \cdot \|w\|_2^2$
- Gradient can simple be decomposed based on the sum rule
- Easy to parallelize/distribute

Basic steps

given a starting point $\boldsymbol{\theta} \in \mathrm{Dom}(f)$
repeat
1. $\Delta\boldsymbol{\theta} := -\nabla f(\boldsymbol{\theta})$
2. Line search. $t^* = \arg\min_{t>0} f(\boldsymbol{\theta} + t \cdot \Delta\boldsymbol{\theta})$
3. Update. $\boldsymbol{\theta} := \boldsymbol{\theta} + t^* \Delta\boldsymbol{\theta}$

until stopping criterion is satisfied.

easy parallel computation

evaluating function might be done multiple times: expensive!

t

1 3 4 2

- Distribute data over several machines
- Compute partial gradients (on each machine in parallel)
- Aggregate the partial gradients to the final one
- BUT: Line search is expensive
  - for each tested step size: scan through all datapoints

Scalability analysis

+ Linear time in number of instances
+ Linear memory consumption in problem size (not data)
+ Logarithmic time in accuracy
+ 'Perfect' scalability

– Multiple passes through dataset for each iteration

A faster algorithm

- Avoid the line search; simply pick update

$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - \tau \cdot \nabla f(\boldsymbol{\theta}_t)$$

  - τ is often called the learning rate

choose optimal

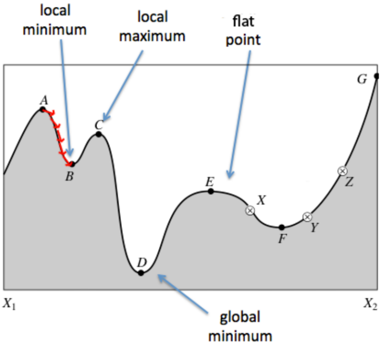
- Only a single pass through data per iteration
- Logarithmic iteration bound (as before)
  - if learning rate is chosen "correctly"

- How to pick the learning rate?
  - too small: slow convergence
  - too high: algorithm might oscillate, no convergence

- Interactive tutorial on optimization
  - http://www.benfrederickson.com/numerical-optimization/

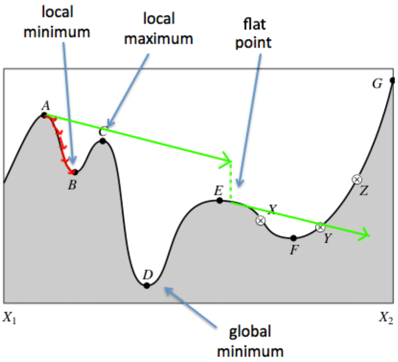
The value of τ

- A too small value for τ has two drawbacks
  - We find the minimum more slowly
  - We end up in local minima or saddle/flat points



The value of τ

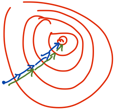
- A too large value for τ has one drawback
  - You may never find a minimum; oscillations usually occur
- We only need 1 step to overshoot



Learning rate adaptation

- Simple solution: let the learning rate be a decreasing function τ_t of the iteration number t
  - so called learning rate schedule
  - first iterations cause large changes in the parameters; later do fine-tuning
  - convergence easily guaranteed if $\lim_{t\to\infty} \tau_t = 0$
  - example: $\tau_{t+1} \leftarrow \alpha \cdot \tau_t$ for $0 < \alpha < 1$

Learning rate adaptation



- Other solutions: Incorporate "history" of previous gradients
- Momentum:

faster

  - $\boldsymbol{m}_t \leftarrow \tau \cdot \nabla f(\boldsymbol{\theta}_t) + \gamma \cdot \boldsymbol{m}_{t-1}$ // often $\gamma = 0.5$
  - $\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - \boldsymbol{m}_t$
  - As long as gradients point to the same direction, the search accelerates
- AdaGrad:
  - different learning rate per parameter
  - learning rate depends inversely on accumulated "strength" of all previously computed gradients
  - large parameter updates ("large" gradients) lead to small learning rates

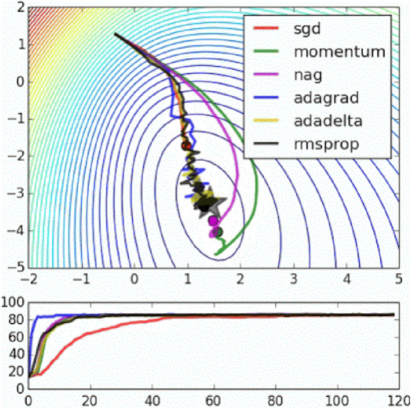
Adaptive moment estimation (Adam)

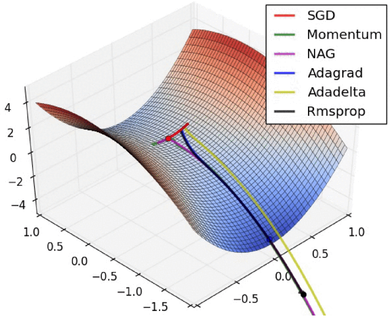
- $\boxed{\boldsymbol{m}_t} = \beta_1 \boxed{\boldsymbol{m}_{t-1}} + (1-\beta_1)\boxed{\nabla f(\boldsymbol{\theta}_t)}$
  - estimate of the first moment (mean) of the gradient
  - Exponentially decaying average of past gradients m_t (similar to momentum)
- $\boxed{\boldsymbol{v}_t} = \beta_2 \boxed{\boldsymbol{v}_{t-1}} + (1-\beta_2)\boxed{(\nabla f(\boldsymbol{\theta}_t))}^2$
  - estimate of the second moment (uncentered variance) of the gradient
  - exponentially decaying average of past squared gradients v_t
- To avoid bias towards zero (due to 0's initialization) use bias-corrected version instead:
  - $\hat{\boldsymbol{m}}_t = \frac{\boldsymbol{m}_t}{1-\beta_1^t} \qquad \hat{\boldsymbol{v}}_t = \frac{\boldsymbol{v}_t}{1-\beta_2^t}$
- Finally, the Adam update rule for parameters θ:
  - $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \frac{\tau}{\sqrt{\hat{\boldsymbol{v}}_t}+\epsilon}\boxed{\hat{\boldsymbol{m}}_t}$
- Default values: $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$

Visualizing gradient descent variants

- AdaGrad and variants
  - often have faster convergence
  - might help to escape saddlepoints

http://sebastianruder.com/optimizing-gradient-descent/



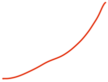


Discussion

- Gradient descent and similar techniques are called first-order optimization techniques
  - they only exploit information of the gradients (i.e. first order derivative)

- Higher-order techniques use higher-order derivatives
  - e.g. second-order = Hessian matrix
  - Example: Newton Method

Newton method



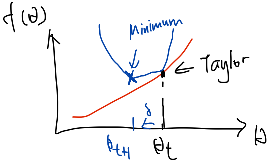
$x^T A x \geq 0$

- Convex objective function f
- Nonnegative second derivative: $\nabla^2 f(\boldsymbol{\theta}) \succeq 0$ // Hessian matrix
  - $\nabla^2 f(\boldsymbol{\theta}) \succeq 0$ means that the Hessian is positive semidefinite

- Taylor expansion of f at point θ_t

$$f(\boldsymbol{\theta}_t + \boldsymbol{\delta}) = f(\boldsymbol{\theta}_t) + \boldsymbol{\delta}^T \nabla f(\boldsymbol{\theta}_t) + \frac{1}{2}\boldsymbol{\delta}^T \nabla^2 f(\boldsymbol{\theta}_t)\boldsymbol{\delta} + O(\boldsymbol{\delta}^3)$$

Newton method



- Convex objective function f
- Nonnegative second derivative: $\nabla^2 f(\boldsymbol{\theta}) \succeq 0$ // Hessian matrix
  - $\nabla^2 f(\boldsymbol{\theta}) \succeq 0$ means that the Hessian is positive semidefinite

- Taylor expansion of f at point θ_t

$$f(\boldsymbol{\theta}_t + \boldsymbol{\delta}) = f(\boldsymbol{\theta}_t) + \boldsymbol{\delta}^T \nabla f(\boldsymbol{\theta}_t) + \frac{1}{2}\boldsymbol{\delta}^T \nabla^2 f(\boldsymbol{\theta}_t)\boldsymbol{\delta} + O(\boldsymbol{\delta}^3) = g(\delta)$$

$\nabla g(\delta) \overset{!}{=} 0$

- Minimize approximation: leads to

$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - [\nabla^2 f(\boldsymbol{\theta}_t)]^{-1} \nabla f(\boldsymbol{\theta}_t)$$

$\Leftrightarrow \delta^* = \text{minimum}_\delta \ldots$

- Repeat until convergence

Parallel Newton method

- + Good rate for convergence
- Faster + Few passes through data needed
- + Parallel aggregation of gradient and Hessian
- + Gradient requires $O(d)$ data

- \- Hessian requires $O(d^2)$ data
- \- Update step is $O(d^3)$ & nontrivial to parallelize To do Inverse $\nabla^2 f(\theta_t)^{-1}$

- Use it only for low dimensional problems!

Large scale optimization

- Higher-order techniques have nice properties (e.g. convergence) but they are prohibitively expensive for high dimensional problems

- For large scale data / high dimensional problems use first-order techniques
  too slow
  - i.e. variants of gradient descent

- But for real-world large scale data even first-order methods are too costly
- Solution: Stochastic optimization!

Motivation: Stochastic Gradient Descent

- Goal: minimize $f(\boldsymbol{\theta}) = \sum_{i=1}^{n} L_i(\boldsymbol{\theta})$ $\quad$ + potential constraints

- For very large data: even a single pass through the data is very costly
- Lots of time required to even compute the very first gradient

- Is it possible to update the parameters more frequently/faster?

Stochastic Gradient Descent

- Consider the task as empirical risk minimization

$$\frac{1}{n}(\sum_{i=1} nL_i(\boldsymbol{\theta})) = \mathop{\mathbb{E}}_{i\sim\{1,\ldots,n\}}[L_i(\boldsymbol{\theta})]$$

- (Exact) expectation can be approximated by smaller sample: = subset
- $\mathbb{E}_{i\sim\{1,\ldots,n\}}[L_i(\boldsymbol{\theta})] \approx \frac{1}{|S|}\sum_{j\in S}(L_j(\boldsymbol{\theta}))$ // with $S \subseteq \{1,\ldots,n\}$

subset

or equivalently: $\sum_{i=1}^{n} L_i(\boldsymbol{\theta}) \approx \boxed{\frac{n}{|S|}} \sum_{j\in \boxed{S}} L_j(\boldsymbol{\theta})$

scaling

Stochastic Gradient Descent

- Intuition: Instead of using "exact" gradient, compute only a noisy (but still unbiased) estimate based on smaller sample

- Stochastic gradient decent:
  1. randomly pick a (small) subset S of the points $\rightarrow$ so called mini-batch
  2. compute gradient based on mini-batch
  3. update: $\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - \tau \cdot \frac{n}{|S|} \cdot \sum_{j \in S} \boldsymbol{\nabla} L_j(\boldsymbol{\theta}_t)$
  4. pick a new subset and repeat with 2

τ: learning rate

$\frac{n}{|S|}$: up-scaling

- "Original" SGD uses mini-batches of size 1
  - larger mini-batches lead to more stable gradients (i.e. smaller variance in the estimated gradient)

- In many cases, the data is sampled so that we don't see any data point twice. Then, each full iteration over the complete data set is called one "epoch".

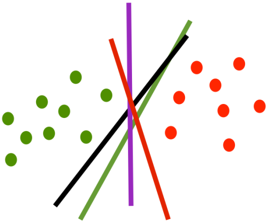
Example: Perceptron

1. model

2. Loss

- Simple linear binary classifier: 1

$$\boxed{\delta(\boldsymbol{x}) = \begin{cases} 1 & \textit{if } \boldsymbol{w}^T\boldsymbol{x} + b > 0 \\ -1 & \textit{else} \end{cases}}$$



- Learning task:
  Given $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ with $y_i \in \{-1, 1\}$
  Find $\min_{\boldsymbol{w},b} \underline{\sum_i L(y_i, \boldsymbol{w}^T\boldsymbol{x}_i + b)}$

- L is the loss function, with $\epsilon > 0$ 2

$$\boxed{\text{- e.g. } L(u,v) = \max(0, \epsilon - u \cdot v) = \begin{cases} \epsilon - uv & \text{if } uv < \epsilon \\ 0 & \text{else } uv \geq \epsilon \end{cases}}$$

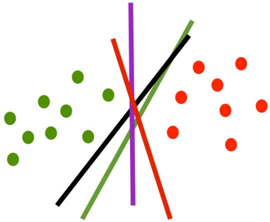
u: grand truth

V: prediction

Example: Perceptron

- Simple linear binary classifier:

$$\delta(\boldsymbol{x}) \begin{cases} 1 & \textit{if } \boldsymbol{w}^T\boldsymbol{x} + b > 0 \\ -1 & \textit{else} \end{cases}$$



- Learning task:
  Given $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ with $y_i\{-1, 1\}$
  Find $\min_{\boldsymbol{w},b} \sum_i L(y_i, \boldsymbol{w}^T\boldsymbol{x}_i + b)$

- L is the loss function, with $\epsilon > 0$

$\epsilon - y_i(w^T x + b)$

  - e.g. $L(u,v) = \max(0, \epsilon - u \cdot v) = \begin{cases} \epsilon - uv & \text{if } uv < \epsilon \quad \leftarrow \textit{incorrect prediction} \\ 0 & \text{else} \quad \leftarrow \textit{correct prediction} \end{cases}$

$\nabla_w L(y_i, w^T x_i + b) = \begin{cases} -y_i \cdot x_i & \text{if } uv \leq \epsilon \\ 0 & \text{Else} \end{cases}$

$\nabla_b L = \begin{cases} -y_i \\ 0 \end{cases}$

Example: Perceptron

$\Theta_{i+1} \leftarrow \Theta_i - \tau \cdot \frac{m}{1} \nabla L.$ if right classify $\nabla L = 0$

- Let's solve this problem via SGD
- Result:

initialize $\boldsymbol{w} = \boldsymbol{0}$ and $b = 0$
repeat
  if $y_i \cdot (\boldsymbol{w}^T \boldsymbol{x}_i + b) < \epsilon$ **then** misclassified
    $\boldsymbol{w} \leftarrow \boldsymbol{w} + \underbrace{\tau \cdot n}_{1} \cdot y_i \cdot \boldsymbol{x}_i$ and $b \leftarrow b + \underbrace{\tau \cdot n}_{1} \cdot y_i$
  end if
until all classified correctly

$\tau = \frac{1}{n}$

- Note: Nothing happens if classified correctly
  - gradient is zero

- Does this remind you of the original learning rules for perceptron?

Convergence in expectation

- Subject to relatively mild assumptions, stochastic gradient descent converges almost surely to a global minimum when the objective function is convex
  - almost surely to a local minimum for non-convex functions

- The expectation of the residual error decreases with speed

$$\mathbb{E}[\rho] \sim t^{-1} \qquad // \text{ i.e. } t \sim \mathbb{E}[\rho]^{-1}$$

residual

$|f(\theta_i) - f(\theta^*)|$

#iteration

- Note: Standard GD has speed $t \sim \log \rho^{-1}$
  - faster convergence speed; but each iteration takes longer

Optimizing Logistic Regression

- Recall we wanted to solve $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} E(\boldsymbol{w})$
- $$E(\boldsymbol{w}) = -\ln p(\boldsymbol{y}|\boldsymbol{w}, \boldsymbol{X})$$ negative log-likelihood $$= -\sum_{i=1}^{N} y_i \ln \sigma(\boldsymbol{w}^T \boldsymbol{x}_i) + (1 - y_i) \ln(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x}_i))$$
- Closed form solution does not exist
- Solution:
  - Compute the gradient $\boldsymbol{\nabla} E(\boldsymbol{w})$
  - Find $\boldsymbol{w}^*$ using gradient descent
- Is $E(\boldsymbol{w})$ convex?
- Can you use SGD?
- How can you choose the learning rate?
- What changes if we add regularization, i.e. $E_{reg}(\boldsymbol{w}) = E(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2$?

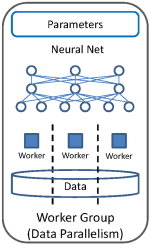
Large-Scale Learning - Distributed Learning

- So far, we (mainly) assumed a single machine
- SGD achieves speed-up by only operating on a subset of the data
  - Might still be too slow when operating with really large data and large models

- In practice: We have often multiple machines available

$\Rrightarrow$ Distributed learning
  - Distribute computation across multiple machines
  - Core challenge: distribute work so that communication doesn't kill you

Distributed Learning: Data vs. Model Parallelism



Use multiple model replicas to process different examples at the same time

- all collaborate to update model state (parameters) in shared parameter server(s)

Many models have lots of inherent parallelism

- local connectivity (as found in CNNs)
- specialized parts of model active only for some examples (see, e.g., Matrix Factorization)

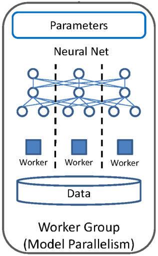


figure based on https://svn.apache.org/repos/infra/websites/production/singa/content/v0.1.0/architecture.html

Parameter Server

- General goal: Keep time to send/receive parameters over network small, compared to the actual time used for computation

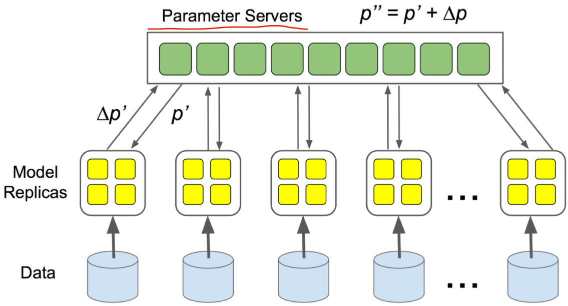


figure from Large Scale Distributed Systems for Training Neural Networks, Jeff Dean

Distributed Learning in Practice

- Distributed optimization/learning is essential when operating with very large data (and large models)
  - Default for training ML models in today's production systems
- Many modern ML frameworks (e.g. Tensorflow, PyTorch, MXNet, ...) provide support for distributed learning
- Many further aspects/challenges
  - Desired synchronization
  - Fault tolerance, recovery
  - Automatic placement (of data/model) to reduce communication

Summary

- General task: Find solution $\boldsymbol{\theta}^*$ minimizing function f
- Convex sets $\&$ functions
  - Global vs. local minimum
  - Verifying convexity: Definition, special results (first-order convexity, 2nd derivative), convexity-preserving operations
- Gradient descent: $\boldsymbol{\theta} := \boldsymbol{\theta} - t\boldsymbol{\nabla} f(\boldsymbol{\theta})$
  - How to choose t? Line search, fixed
  - Learning rate: Fix $t = \tau$; or use an adaptive learning rate (momentum, AdaGrad, Adam)
  - Stochastic gradient descent (SGD): Only use part of data (mini-batches) at each step
- Distributed Learning: exploit multiple machines
  - data parallelism, model parallelism

Reading material

Reading material

- Boyd - Convex Optimization: chapters 2.1-2.3, 3.1, 3.2, 4.1, 4.2, 9
  - free PDF version online
- Sebastian Ruder - An overview of gradient descent optimization algorithms
  - https://arxiv.org/abs/1609.04747