Machine Learning

Lecture 6: Optimization

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Motivation

- Many machine learning tasks are optimization problems
- Examples we've already seen:
  - Linear Regression $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \frac{1}{2}(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^T(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$
  - Logistic Regression $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} -\ln p(\boldsymbol{y} \mid \boldsymbol{w}, \boldsymbol{X})$
- 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

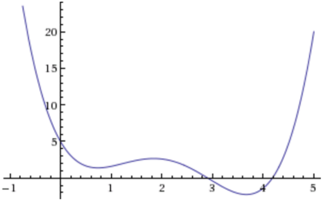
- Let $\boldsymbol{\theta}$ denote the variables/parameters of our problem we want to learn
  - e.g. $\boldsymbol{\theta} = \boldsymbol{w}$ in Logistic Regression
- Let $\mathcal{X}$ denote the domain of $\boldsymbol{\theta}$; the set of valid instantiations
  - constraints on the parameters!
  - e.g. $\mathcal{X} =$ 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

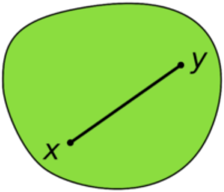
- Necessary condition for minima
  - Gradient = 0
  - Sufficient?

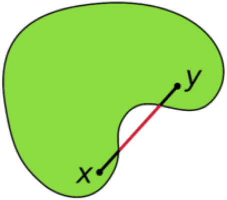


- General challenge: multiple local minima possible

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 $\lambda \in [0, 1]$



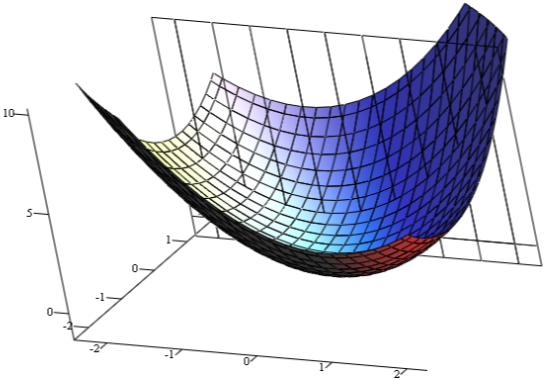


Convexity: Functions

- $f(\boldsymbol{x})$ 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 $\lambda \in [0,1]$



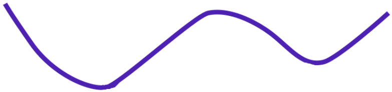
Convexity and *minimization problems*

- 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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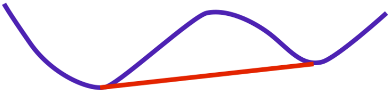

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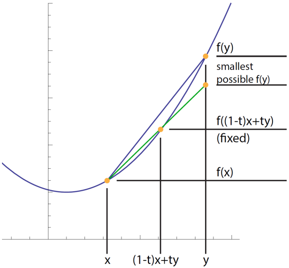
First order convexity conditions (I)

- 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)

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

- 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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2. Exploit special results

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- 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)

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)

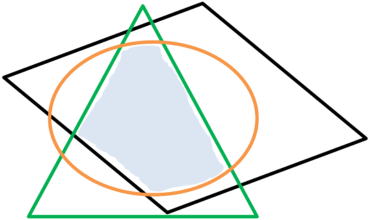
Convexity preserving operations

- 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: $e^{x_1 + 2 * x_2} + x_1 - \log(x_2)$ 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



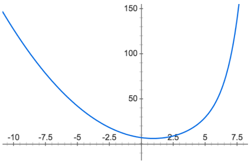
An easy problem

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

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

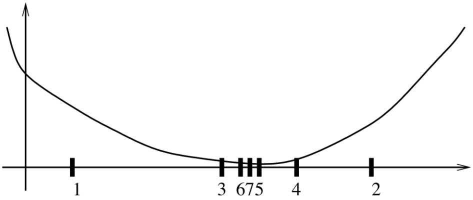


Outlook

- 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

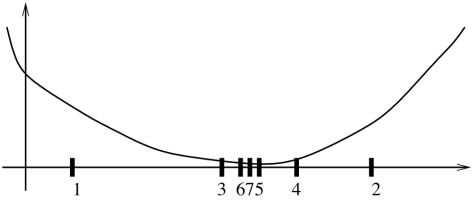
until

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

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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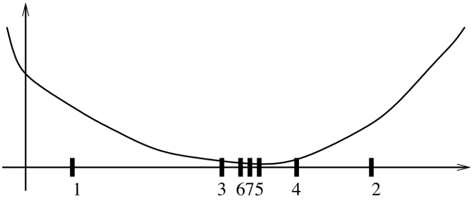
One-dimensional problems

- 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



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

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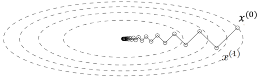
solution on the left

Gradient Descent

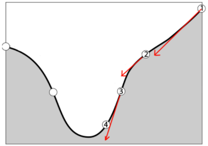
- Key Idea
  - Gradient points into steepest ascent direction
  - Locally, the gradient is a good approximation of the objective function



- 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.



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

- Linear convergence for strongly convex objective
  - $k \sim \log(\rho^{-1})$ // $k =$ 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
  - $L_i(\boldsymbol{w}) = (\boldsymbol{x}_i^T \boldsymbol{w} - y_i)^2$ $\quad g(\boldsymbol{w}) = \lambda \cdot \|w\|_2^2$
- 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. $\Delta\boldsymbol{\theta} := -\nabla f(\boldsymbol{\theta})$
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until stopping criterion is satisfied.

easy parallel computation

evaluating function might be done multiple times: expensive!

- 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

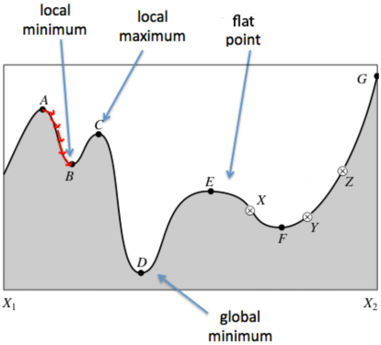
- Only a single pass through data per iteration
- Logarithmic iteration bound (as before)
  - if learning rate is chosen "correctly"

- 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/

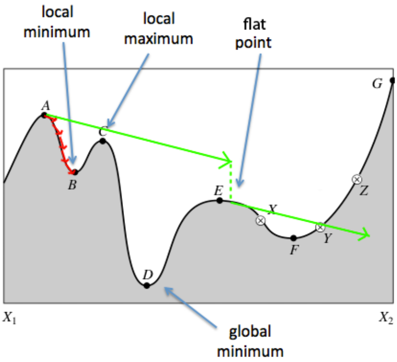
The value of τ

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

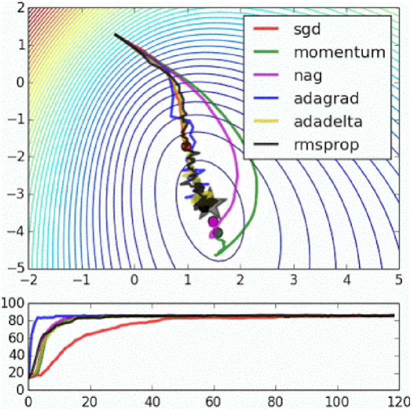
Adaptive moment estimation (Adam)

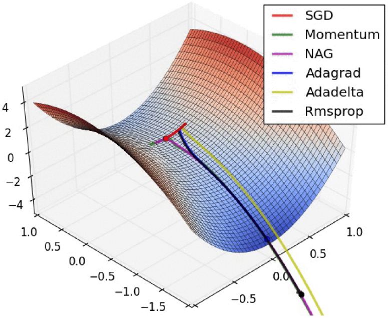
- $\boldsymbol{m}_t = \beta_1 \boldsymbol{m}_{t-1} + (1 - \beta_1) \nabla f(\boldsymbol{\theta}_t)$
  - estimate of the first moment (mean) of the gradient
  - Exponentially decaying average of past gradients m_t (similar to momentum)
- $\boldsymbol{v}_t = \beta_2 \boldsymbol{v}_{t-1} + (1 - \beta_2)(\nabla f(\boldsymbol{\theta}_t))^2$
  - 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:
  - $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \frac{\tau}{\sqrt{\hat{\boldsymbol{v}}_t}+\epsilon} \hat{\boldsymbol{m}}_t$
- 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

- 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: $\boldsymbol{\nabla}^2 f(\boldsymbol{\theta}) \succeq 0$ // Hessian matrix
  - $\boldsymbol{\nabla}^2 f(\boldsymbol{\theta}) \succeq 0$ means that the Hessian is positive semidefinite
- Taylor expansion of f at point θ_t

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

- Minimize approximation: leads to

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

- Repeat until convergence

Parallel Newton method

- + Good rate for convergence
- + 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

- 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
  - 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 $f(\boldsymbol{\theta}) = \sum_{i=1}^{n} L_i(\boldsymbol{\theta}) \qquad +$ 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

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

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

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

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

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

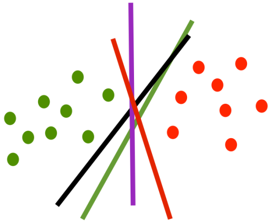
- In many cases, the data is sampled so that we don't see any data point twice. Then, each full iteration over the complete data set is called one "epoch".

Example: Perceptron

- 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 $y_i \in \{-1, 1\}$
  Find $\min_{\boldsymbol{w},b} \sum_i L(y_i, \boldsymbol{w}^T\boldsymbol{x}_i + b)$



- L is the loss function, with $\epsilon > 0$
  - e.g. $L(u, v) = \max(0, \epsilon - u \cdot v) = \begin{cases} \epsilon - uv & \text{if } uv < \epsilon \\ 0 & \text{else} \end{cases}$

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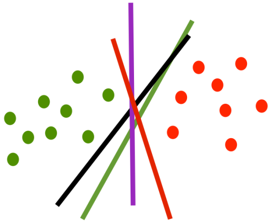

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Example: Perceptron

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

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

- 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

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

- 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 $\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} E(\boldsymbol{w})$
- $E(\boldsymbol{w}) = -\ln p(\boldsymbol{y}|\boldsymbol{w}, \boldsymbol{X})$

$$= -\sum_{i=1}^{N} y_i \ln \sigma(\boldsymbol{w}^T \boldsymbol{x}_i) + (1 - y_i) \ln(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x}_i))$$

- 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. $E_{reg}(\boldsymbol{w}) = E(\boldsymbol{w}) + \lambda \|\boldsymbol{w}\|_2^2$?

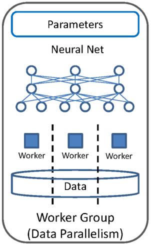
Large-Scale Learning - Distributed Learning

- 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)

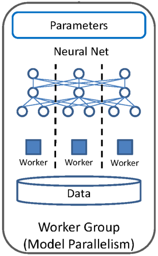


figure based on https://svn.apache.org/repos/infra/websites/production/singa/content/v0.1.0/architecture.html

Parameter Server

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

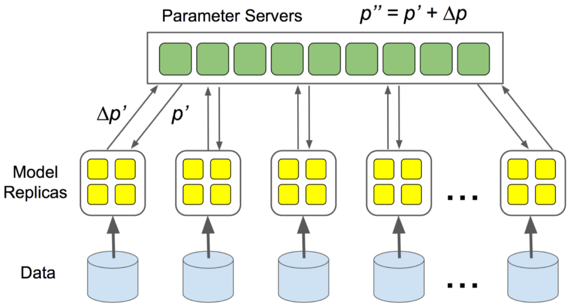


figure from Large Scale Distributed Systems for Training Neural Networks, Jeff Dean

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