Local, Unconstrained Function Optimization

COMPSCI 371D — Machine Learning

Outline

Motivation and Scope

- Most estimation problems are solved by optimization
- Machine learning:
  - Parametric predictor: $h(\mathbf{x}\ ;\ \mathbf{v})\ :\ \mathbb{R}^d \times \mathbb{R}^m \to Y$
  - Training set $T = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$ and *loss* = $\ell(y_n, y)$
  - Risk: $L_T(\mathbf{v}) = \frac{1}{N}\sum_{n=1}^{N} \ell(y_n, h(\mathbf{x}_n\ ;\ \mathbf{v}))\ :\ \mathbb{R}^m \to \mathbb{R}$
  - Training: $\hat{\mathbf{v}} \in \arg\min_{\mathbf{v}\in\mathbb{R}^m} L_T(\mathbf{v})$
- "Solving" the system of equations $\mathbf{e}(\mathbf{z}) = \mathbf{0}$ can be viewed as

  $$\hat{\mathbf{z}} =\in \arg\min_{\mathbf{z}} \|\mathbf{e}(\mathbf{z})\|$$

Only *Local* Minimization

$\hat{\mathbf{z}} = \arg\min_{\mathbf{z} \in ?} f(\mathbf{z})$

- All we know about f is a “black box” (think Python function)
- For many problems, f has many local minima
- Start somewhere ($\mathbf{z}_0$), and take steps “down”

  $f(\mathbf{z}_{k+1}) < f(\mathbf{z}_k)$
- When we get stuck at a local minimum, we declare success
- We would like global minima, but all we get is local ones
- For some problems, f has a unique minimum...
- ... or at least a single connected set of minima

Gradient

$$\nabla f(\mathbf{z}) = \frac{\partial f}{\partial \mathbf{z}} = \begin{bmatrix} \frac{\partial f}{\partial z_1} \\ \vdots \\ \frac{\partial f}{\partial z_m} \end{bmatrix}$$

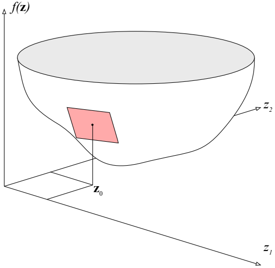
$\mathbf{z} \in \mathbb{R}^m$ with m possibly very large

- If $\nabla f(\mathbf{z})$ exists everywhere, the condition $\nabla f(\mathbf{z}) = \mathbf{0}$ is necessary and sufficient for a stationary point (max, min, or saddle)
- Warning: only *necessary* for a minimum!
- Reduces to first derivative when $f : \mathbb{R} \to \mathbb{R}$

First Order Taylor Expansion

$$f(\mathbf{z}) \approx g_1(\mathbf{z}) = f(\mathbf{z}_0) + [\nabla f(\mathbf{z}_0)]^T(\mathbf{z} - \mathbf{z}_0)$$

approximates $f(\mathbf{z})$ near $\mathbf{z}_0$ with a (hyper)plane through $\mathbf{z}_0$



$\nabla f(\mathbf{z}_0)$ points to direction of steepest *increase* of f at $\mathbf{z}_0$

- If we want to find $\mathbf{z}_1$ where $f(\mathbf{z}_1) < f(\mathbf{z}_0)$, going along $-\nabla f(\mathbf{z}_0)$ seems promising
- This is the general idea of *gradient descent*

Hessian

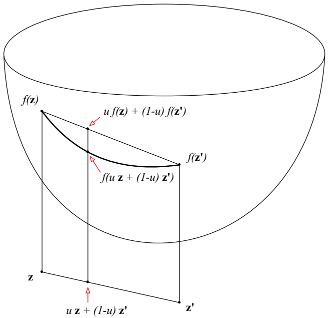
$$H(\mathbf{z}) = \begin{bmatrix} \frac{\partial^2 f}{\partial z_1^2} & \cdots & \frac{\partial^2 f}{\partial z_1 \partial z_m} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial z_m \partial z_1} & \cdots & \frac{\partial^2 f}{\partial z_m^2} \end{bmatrix}$$

- Symmetric matrix because of Schwarz's theorem:

$$\frac{\partial^2 f}{\partial z_i \partial z_j} = \frac{\partial^2 f}{\partial z_j \partial z_i}$$

- Eigenvalues are real because of symmetry
- Reduces to $\frac{d^2 f}{dz^2}$ for $f : \mathbb{R} \to \mathbb{R}$

Convexity



- Weakly convex *everywhere*:
  For all $\mathbf{z}, \mathbf{z}'$ in the (open) domain of f and for all $u \in (0, 1)$
  $f(u\mathbf{z} + (1-u)\mathbf{z}') \;\leq\; uf(\mathbf{z}) + (1-u)f(\mathbf{z}')$
- Strong convexity: Replace "$\leq$" with"$<$"

Convexity and Hessian

- Things become operational for twice-differentiable functions
- The function $f(\mathbf{z})$ is weakly convex everywhere iff $H(\mathbf{z}) \succeq 0$ for all $\mathbf{z}$
- "$\succeq$" means *positive semidefinite*:
  $\mathbf{v}^T H(\mathbf{z})\mathbf{v} \;\geq\; 0$ for all $\mathbf{v} \in \mathbb{R}^m$
- Above is *definition* of $H(\mathbf{z}) \succeq 0$
- To check computationally: All eigenvalues are nonnegative
- $H(\mathbf{z}) \succeq 0$ reduces to $\frac{d^2 f}{dz^2} \geq 0$ for $f \;:\; \mathbb{R} \to \mathbb{R}$
- Analogous result for strong convexity: $H(\mathbf{z}) \succ 0$, that is,
  $\mathbf{v}^T H(\mathbf{z})\mathbf{v} \;>\; 0$ for all $\mathbf{v} \in \mathbb{R}^m$
  (All eigenvalues are positive)

Local Convexity

- The function f is convex *at* $\mathbf{z}_0$ if it is convex everywhere in some open neighborhood of $\mathbf{z}_0$
- Convexity at $\mathbf{z}_0$ is *not* equivalent to $H(\mathbf{z}_0) \succ 0$ or $H(\mathbf{z}_0) \succcurlyeq 0$
  - $H(\mathbf{z}_0) \succ 0$ is only *sufficient* for strong convexity at $\mathbf{z}_0$
    - Example: $f(z) = x^2/2$ is strongly convex at $z_0 = 0$ and $H_f(z_0) = 1 \succ 0$
    - Example: $f(z) = x^4$ is strongly convex at $z_0 = 0$ but $H_f(z_0) = 0 \not\succ 0$ (so $H_f(z_0) = 1 \succ 0$ is not necessary for strong convexity at z_0)
  - For weak convexity at $\mathbf{z}_0$ we need to check that $H(\mathbf{z}) \succcurlyeq 0$ *for every* $\mathbf{z}$ *in some open neighborhood of* $\mathbf{z}_0$
  - Example: $f(z) = z^3/6$, for which we have $H_f(z) = z$
    - $H_f(0) \succcurlyeq 0$ (and in fact $H_f(0) = 0$)
    - However, every neighborhood of $z_0 = 0$ has points (any $z < 0$) where $H_f(z) \prec 0$
    - So $f(z)$ is not (even weakly) convex at $z_0 = 0$

Some Uses of Convexity

- If $\nabla f(\hat{\mathbf{z}}) = \mathbf{0}$ and f is convex at $\hat{\mathbf{z}}$ then $\hat{\mathbf{z}}$ is a minimum (as opposed to a maximum or a saddle)
- If f is globally convex then the value of the minimum is unique and minima form a convex set
- Faster optimization methods can be used when $f : \mathbb{R}^m \rightarrow \mathbb{R}$ is convex and m is not too large

A Template for Local Minimization

- Regardless of method, most local unconstrained optimization methods fit the following template:

  $k = 0$
  while $\mathbf{z}_k$ is not a minimum
  compute step direction $\mathbf{p}_k$
  compute step size $\alpha_k > 0$
  $\mathbf{z}_{k+1} = \mathbf{z}_k + \alpha_k \mathbf{p}_k$
  $k = k + 1$
  end

- For some methods the *step*

$$\mathbf{s}_k = \mathbf{z}_{k+1} - \mathbf{z}_k = \alpha_k \mathbf{p}_k$$

  is the result of a single computation

Design Decisions

$k = 0$
while $\mathbf{z}_k$ is not a minimum
    compute step direction $\mathbf{p}_k$
    compute step size $\alpha_k > 0$
    $\mathbf{z}_{k+1} = \mathbf{z}_k + \alpha_k \mathbf{p}_k$
    $k = k + 1$
end

- In what direction to proceed ($\mathbf{p}_k$)
- How long a step to take in that direction (α_k)
- When to stop ("while $\mathbf{z}_k$ is not a minimum")
- Different decisions lead to different methods

Gradient Descent

- In what direction to proceed: $\mathbf{p}_k = -\nabla f(\mathbf{z}_k)$
- "Gradient descent"
- Problem reduces to one dimension: $h(\alpha) = f(\mathbf{z}_k + \alpha \mathbf{p}_k)$
- $\alpha = 0 \Leftrightarrow \mathbf{z} = \mathbf{z}_k$
- Find $\alpha = \alpha_k > 0$ such that $f(\mathbf{z}_k + \alpha_k \mathbf{p}_k) < f(\mathbf{z}_k)$
- How to find α_k?

Stochastic Gradient Descent

- A special case of gradient descent, SGD works for *averages* of many terms (N very large):

$$f(\mathbf{z}) = \frac{1}{N} \sum_{n=1}^{N} \phi_n(\mathbf{z})$$

- Computing $\nabla f(\mathbf{z}_k)$ is too expensive
- Partition $B = \{1, \ldots, N\}$ into J random *mini-batches* B_j each of about equal size

$$f(\mathbf{z}) \approx f_j(\mathbf{z}) = \frac{1}{|B_j|} \sum_{n \in B_j} \phi_n(\mathbf{z}) \quad \Rightarrow \quad \nabla f(\mathbf{z}) \approx \nabla f_j(\mathbf{z}) \; .$$

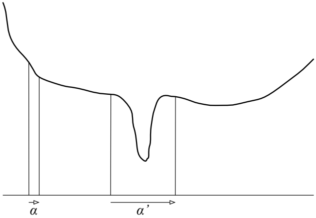
- Mini-batch gradients are correct *on average*

SGD and Mini-Batch Size

- SGD iteration: $\mathbf{z}_{k+1} = \mathbf{z}_k - \alpha_k \nabla f_j(\mathbf{z}_k)$
- Mini-batch gradients are correct *on average*
- One cycle through all the mini-batches is an *epoch*
- Repeatedly cycle through all the data
  (Scramble data before each epoch)
- *Asymptotic* convergence can be proven with suitable step-size schedule
- Small batches $\Rightarrow$ low storage but high gradient variance
- Make batches as big as will fit in memory for minimal variance
- In deep learning, memory is GPU memory

Step Size

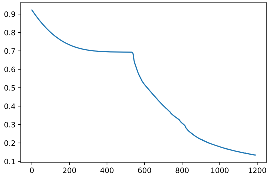
- Simplest idea: $\alpha_k = \alpha$ (fixed)
  - Small α leads to slow progress
  - Large α can miss minima



- Scheduling α:
  - Start with α relatively large (say $\alpha = 10^{-3}$)
  - Decrease α over time
  - Determine decrease rate by trial and error

Momentum

- Sometimes $\mathbf{z}_k$ meanders around in shallow valleys



$f(\mathbf{z}_k)$ versus k

- α is too small, direction is still promising
- Add *momentum*

$$\mathbf{v}_0 = \mathbf{0}$$

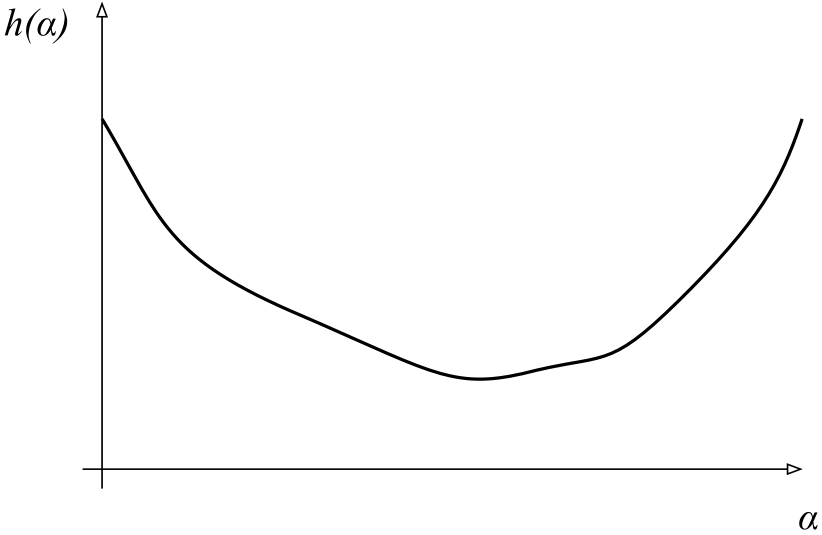
$$\mathbf{v}_{k+1} = \mu_k \mathbf{v}_k - \alpha \nabla f(\mathbf{z}_k) \qquad (0 \leq \mu_k < 1)$$

$$\mathbf{z}_{k+1} = \mathbf{z}_k + \mathbf{v}_{k+1}$$

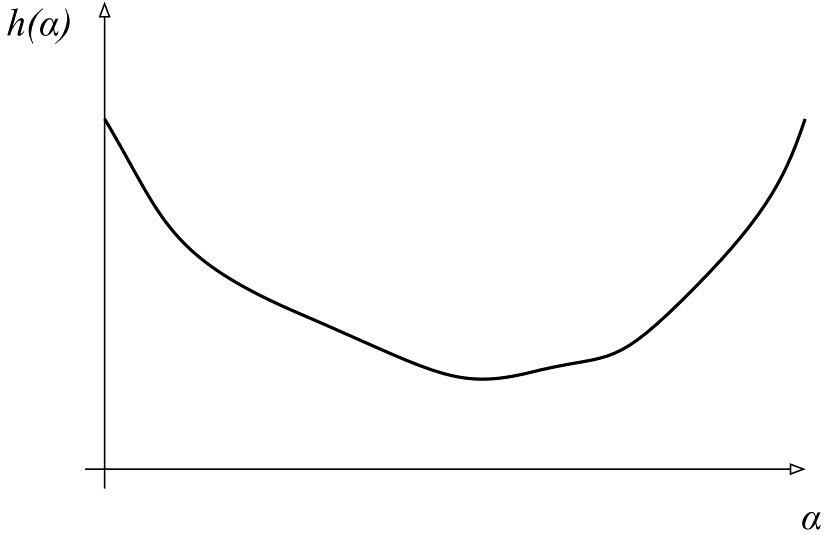
Line Search

- Find a local minimum in the search direction $\mathbf{p}_k$
  $h(\alpha) = f(\mathbf{z}_k + \alpha\mathbf{p}_k)$, a one-dimensional problem
- *Bracketing triple*:
- $a < b < c, \quad h(a) \geq h(b), \quad h(b) \leq h(c)$
- Contains a (local) minimum!
- Split the bigger of $[a, b]$ and $[b, c]$ in half with a point u
- Find a new, narrower bracketing triple involving u and two out of a, b, c
- Stop when the bracket is narrow enough (say, 10^{-6})
- Pinned down a minimum to within 10^{-6}

Phase 1: Find a Bracketing Triple



Phase 2: Shrink the Bracketing Triple



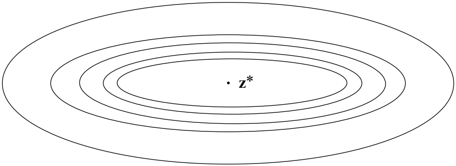
if $b - a > c - b$
    $u = (a + b)/2$
    if $h(u) > h(b)$
        $(a, b, c) = (u, b, c)$
    otherwise
        $(a, b, c) = (a, u, b)$
    end
otherwise
    $u = (b + c)/2$
    if $h(u) > h(b)$
        $(a, b, c) = (a, b, u)$
    otherwise
        $(a, b, c) = (b, u, c)$
    end
end

Termination

- Are we still making “significant progress”?
- Check $f(\mathbf{z}_{k-1}) - f(\mathbf{z}_k)$? (We want this to be strictly positive)
- Check $\|\mathbf{z}_{k-1} - \mathbf{z}_k\|$? (We want this to be large enough)
- Second is more stringent close the the minimum because $\nabla f(\mathbf{z}) \approx \mathbf{0}$
- Stop when $\|\mathbf{z}_{k-1} - \mathbf{z}_k\| < \delta$

Is Gradient Descent a Good Strategy?

- "We are going in the direction of fastest descent"
- "We choose an optimal step size by line search"
- "Must be good, no?" *Not so fast!*
- An example for which we know the answer:
  $f(\mathbf{z}) = c + \mathbf{a}^T\mathbf{z} + \frac{1}{2}\mathbf{z}^T Q\mathbf{z}$
  $Q \succcurlyeq 0$ (convex paraboloid)
- All smooth functions look like this close enough to $\mathbf{z}^*$



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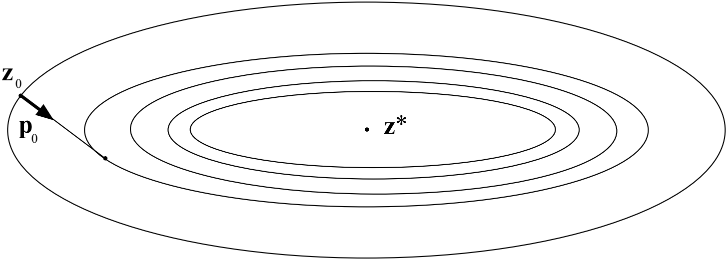
Skating to a Minimum



- Many 90-degree turns slow down convergence
- There are methods that take fewer iterations, but each iteration takes more time and space
- We will stick to gradient descent
- See appendices in the notes for more efficient methods for problems in low-dimensional spaces