Optimization in General - (i.e, not just Deep Learning)

A/Prof Richard Yi Da Xu
http://richardxu.com

University of Technology Sydney (UTS)

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Gradient Descend: what is directional derivative

- **Your aim** to find:

$$\arg\min_{\mathbf{x}} \left(f(\mathbf{x})\right)$$

- How? Solve $\nabla f(\mathbf{x}_n) = 0$! But in many scenarios, this isn't easy!
- The rate of change of $f(x, y)$ in the direction of the unit vector $u = (a, b)$ is called the directional derivative $\mathrm{d}_u f(x, y)$. The definition of the directional derivative is:

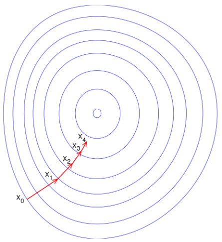
$$\mathrm{d}_u f(x, y) = \lim_{h \to 0} \frac{f(x + ah, y + bh) - f(x, y)}{h}$$

- **Theorem** the minimum directional derivative of a differentiable function f at (x_0, y_0) is $-|\triangledown f(x_0, y_0)|$ and occurs for u with the opposite direction as $\triangledown f(x_0, y_0)$

Gradient Descend

Here is where **Gradient Descend** algorithm may help. The iterative algorithm looks something like:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \nabla f(\mathbf{x}_n), \qquad n \geq 0$$



Moral of the story, you must know how to compute the objective function's **derivative**.

Newton methods

- taylor expansion of $f(\mathbf{x})$ around $\mathbf{x}_n$ in 1-D:

$$f(x_n + \Delta x) \approx f(x_n) + f'(x_n)\Delta x + \frac{1}{2} f''(x_n)\Delta x^2$$

- we need to find what is the "right" value of Δx that minimises $f(.)$:

$$\begin{aligned}
\frac{\mathrm{d}f(x_n + \Delta x)}{\mathrm{d}\Delta x} &= \frac{\mathrm{d}}{\mathrm{d}\Delta x}\left(f(x_n) + f'(x_n)\Delta x + \frac{1}{2} f''(x_n)\Delta x^2 \right) = f'(x_n) + f''(x_n)\Delta x \\
f'(x_n) + f''(x_n)\Delta x = 0 &\implies \Delta x = \frac{-f'(x_n)}{f''(x_n)} \\
x_{n+1} &= x_n + \Delta x \\
&= x_n - (f''(x_n))^{-1} f'(x_n)
\end{aligned}$$

- taylor expansion of $f(\mathbf{x})$ around $\mathbf{x}_n$ in higher dimension:

$$\implies \mathbf{x}_{n+1} = \mathbf{x}_n - \underbrace{\left(\nabla^2 f(\mathbf{x}_n)\right)^{-1}}_{\alpha n} \nabla f(\mathbf{x}_n)$$

Newton methods (2)

- knowing,

$$
\begin{aligned}
\frac{\mathrm{d}f(\mathbf{x}_n + \Delta x)}{\mathrm{d}\Delta\mathbf{x}} &= \mathbf{0} \\
\implies \mathbf{x}_{n+1} &= \mathbf{x}_n - \underbrace{\left(\nabla^2 f(\mathbf{x}_n)\right)^{-1}}_{\alpha_n} \nabla f(\mathbf{x}_n)
\end{aligned}
$$

- $\nabla^2 f(\mathbf{x}_n)$ is called Hessian matrix.
- **bigger** steps in low-curvature (where $\nabla^2 f(\mathbf{x}_n)$ is small)
- **smaller** steps in high-curvature scenarios.

Conjugate Gradient Descend - **why need conjugate?**

- we have a 2-d function $f(x_1, x_2)$:
- suppose step k occurred along x_1-axis, and led to position $\mathbf{x}^{k+1}$
- at $\mathbf{x}^{k+1}$, $f(\mathbf{x}^{k+1})$ is minimized in its x_1 component:

$$\frac{\partial f(\mathbf{x}^{k+1})}{\partial x_1} = 0$$

- next step is along x_2-axis: that step leads to a position $\mathbf{x}^{k+2}$: we find the appropate step, such that:

$$\frac{\partial f(\mathbf{x}^{k+2})}{\partial x_2} = 0$$

- we know $\frac{\partial^2 f(\mathbf{x}^{k+2})}{\partial x_1 \, \partial x_2} = \frac{\partial}{\partial x_2}\left(\frac{\partial f(\mathbf{x}^{k+2})}{\partial x_1}\right)$, then:

$$\frac{\partial^2 f(\mathbf{x}^{k+2})}{\partial x_2 \partial x_1} \neq 0 \implies \frac{\partial f(\mathbf{x}^{k+2})}{\partial x_1} \neq 0$$

- in words, it says if $\mathbf{x}^{k+2}$ is **not** overall stationery/saddle point, and we also know $\mathbf{x}^{k+2}$ **is** stationery point in x_2 direction; then it **mustn't** be stationery point in x_1 direction
- we want to move along direction other than x_2-axis, such that $\frac{\partial f(\mathbf{x}^{k+2})}{\partial x_1}$ remains zero

Q-conjugate

- the next four slides are heavily referenced using `http://www.cs.cmu.edu/~pradeepr/convexopt/Lecture_Slides/conjugate_direction_methods.pdf`
- we need to search for new non-axis directions:
- $\{d_1, d_2, \dots, d_n\}$ are said to be Q-conjugate, such that,

$$d_j^\top Q d_k = 0 \qquad j \neq k$$

- when Q is also symmetric, $\{\lambda_k, v_k\}$ are eigen-(value,vector) pair, we know all eigen-vectors are orthogonal:

$$\begin{aligned} Q v_k &= \lambda_k v_k \\ \implies v_j^\top Q v_k &= \lambda_k v_j^\top v_k = 0 \qquad j \neq k \end{aligned}$$

- so eigen-vectors $\{v_1, \dots v_n\}$ of symmetric matrix can be thought as special case of Q-conjugate vectors, where these vectors are ortho-normal without Q

CGD: Linear independence

- let Q be **positive definite**, then all its Q-conjugate vectors $\{d_1, d_2, \dots, d_n\}$ are linearly independent
- **proof by contradiction**, i.e., suppose one of its vector say d_k can be written in linear combination of $d_1, \dots, d_{k-1}$:

$$
\begin{aligned}
d_k &= \alpha_1 d_1 + \dots + \alpha_{k-1} d_{k-1} \\
\implies \quad d_k^\top Q d_k &= d_k^\top Q \left(\alpha_1 d_1 + \dots + \alpha_{k-1} d_{k-1}\right) \\
&= d_k^\top Q \alpha_1 d_1 + \dots + d_k^\top Q \alpha_{k-1} d_{k-1} \\
&= 0
\end{aligned}
$$

contradiction part is, by definition of positive definiteness: $d_k^\top Q d_k > 0 \; \forall d_k \neq 0$!

compute α_k independently

- if we are to minimize a **quadratic** problem:

$$\min_{\mathbf{x}\in\mathbb{R}^n} \frac{1}{2}\mathbf{x}^\top Q\mathbf{x} - b^\top \mathbf{x} + c$$

- if matrix $Q \in \mathbb{R}^{n\times n}$ is positive definite, then minimal value $\mathbf{x}^*$ is:

$$Q\mathbf{x}^* = b$$

- let $\{d_0, d_1, \dots, d_{n-1}\}$ be arbitary Q-conjugate set

$$\begin{aligned} \mathbf{x}^* &= \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1} && \text{linearly-independent basis} \\ \implies d_k^\top Q\mathbf{x}^* &= d_k^\top Q\left(\alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}\right) && \times \text{ by arbitrary } k^{\text{th}} \\ &= \alpha_k d_k^\top Q d_k \\ \implies \alpha_k &= \frac{d_k^\top Qx^*}{d_k^\top Q d_k} = \frac{d_k^\top b}{d_k^\top Q d_k} \end{aligned}$$

- **beauty** is that we don't need to know $\mathbf{x}^*$ to compute α_k, only Q-conjugacy is required

Conjugate Direction

$$
\begin{aligned}
\mathbf{x}^* &= \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1} \\
&= \sum_{k=0}^{d-1} \frac{d_k^\top b}{d_k^\top Q d_k} d_k \qquad \text{substitute } \alpha_k = \frac{d_k^\top b}{d_k^\top Q d_k}
\end{aligned}
$$

- the above can be achieved in parallel, where each d_k does **not** minimizing anything
- also it is **not** an algorithm, it simply decomposes $\mathbf{x}^*$
- instead, we try to solve along a **path**, with an initial point $\mathbf{x}^0$:

$$
\begin{aligned}
\mathbf{x}_1 &= \mathbf{x}_0 + \alpha_0 d_0 \\
&\cdots \\
\mathbf{x}_k &= \mathbf{x}_0 + \alpha_0 d_0 + \cdots + \alpha_{k-1} d_{k-1} \\
&\cdots \\
\mathbf{x}^* &= \mathbf{x}_0 + \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}
\end{aligned}
$$

- what about the new α_k to match with this path?

now we have $\mathbf{x}_0$

- $\mathbf{x}_0 \in \mathbb{R}^n$ be an arbitrary starting point:
- so instead of writing $\mathbf{x}^* = \sum_{k=0}^{d-1} \alpha_k d_k$
- we also know $g_k \equiv \nabla f(\mathbf{x}_k) = Q\mathbf{x}_k - b = Q\mathbf{x}_k - Q\mathbf{x}^* = Q(\mathbf{x}_k - \mathbf{x}^*)$
- instead of decompose $\mathbf{x}^*$, let's now try to decompose $\mathbf{x}^* - \mathbf{x}_0$:

$$\mathbf{x}_1 - \mathbf{x}_0 = \underbrace{\mathbf{x}_0 + \alpha_0 d_0}_{\mathbf{x}_1} - \mathbf{x}_0$$

$$\mathbf{x}_k - \mathbf{x}_0 = \underbrace{\mathbf{x}_0 + \alpha_0 d_0 + \cdots + \alpha_k d_{k-1}}_{\mathbf{x}_k} - \mathbf{x}_0 = \alpha_0 d_0 + \cdots + \alpha_{k-1} d_{k-1}$$

$$\mathbf{x}^* - \mathbf{x}_0 = \underbrace{\mathbf{x}_0 + \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}}_{\mathbf{x}^*} - \mathbf{x}_0 = \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}$$

$$\begin{aligned}
\implies d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0) &= d_k^\top Q\left(\alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}\right) \\
&= d_k^\top Q \alpha_k d_k \\
\implies \alpha_k &= \frac{\color{red}{d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0)}}{d_k^\top Q d_k} \\
&= -\frac{d_k^\top g_0}{d_k^\top Q d_k}
\end{aligned}$$

- **recap**, for $\mathbf{x}^* = \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}$:

$$\mathbf{x}^* = \sum_{k=0}^{d-1} \underbrace{\frac{d_k^\top b}{d_k^\top Q d_k}}_{\alpha_k} d_k$$

- **recap**, for $\mathbf{x}^* = \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1} + \mathbf{x}_0$:

$$\mathbf{x}^* - \mathbf{x}_0 = \sum_{k=0}^{d-1} \underbrace{-\frac{d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0)}{d_k^\top Q d_k}}_{\alpha_k} d_k$$

$$\mathbf{x}^* = \sum_{k=0}^{d-1} \underbrace{-\frac{d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0)}{d_k^\top Q d_k}}_{\alpha_k} d_k + \mathbf{x}_0$$

- we will see that to write α_k in terms of $Q(\mathbf{x}^* - \mathbf{x}_0)$ may **not** be as useful as to write in terms of $\mathbf{x}_k$

Expanding subspace theorem

- looking at:

$$\begin{aligned} d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0) &= d_k^\top Q(\mathbf{x}^* - \mathbf{x}_k + \mathbf{x}_k - \mathbf{x}_0) = d_k^\top Q(\mathbf{x}^* - \mathbf{x}_k) + d_k^\top Q(\mathbf{x}_k - Q\mathbf{x}_0) \\ &= d_k^\top Q(\mathbf{x}^* - \mathbf{x}_k) + d_k^\top Q\left(\alpha_0 d_0 + \dots + \alpha_{n-1} d_{n-1}\right) \\ &= d_k^\top Q(\mathbf{x}^* - \mathbf{x}_k) \end{aligned}$$

- noted that $d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0) = d_k^\top Q(\mathbf{x}^* - \mathbf{x}_k) \not\Longrightarrow Q(\mathbf{x}^* - \mathbf{x}_0) = Q(\mathbf{x}^* - \mathbf{x}_k)$
- think about the case:

$$[1 \quad 1]\, v_1 = [1 \quad 1]\, v_2 = 5 \quad \text{but} \quad v_1 = [4 \quad 1] \text{ and } v_2 = [1 \quad 4] \text{ satisfy}$$

- therefore:

$$\alpha_k = \frac{d_k^\top Q(\mathbf{x}^* - \mathbf{x}_0)}{d_k^\top Q d_k} = -\frac{d_k^\top g_0}{d_k^\top Q d_k} = \frac{d_k^\top Q(\mathbf{x}^* - \mathbf{x}_k)}{d_k^\top Q d_k} = -\frac{d_k^\top g_k}{d_k^\top Q d_k}$$

- **recap**: we move from $\mathbf{x}_0$ by adding Q-conjugate directions $\{d_1, \dots d_n\}$, each time by $\alpha_k = -\frac{d_k^\top g_k}{d_k^\top Q d_k}$ amount
- we need to prove why this movement is getting “better”, i.e., each k step **minimizes all previous directions**

Looking at the algorithm closely

- to know if $\mathbf{x}_k$ is minimizing dimensions along its path using step size $\alpha_k = -\frac{d_k^\top g_k}{d_k^\top Q d_k}$:

$$\mathbf{x}_k \xrightarrow{\alpha_k \times d_k} \mathbf{x}_{k+1} \qquad \mathbf{x}_{k+1} \xrightarrow{\alpha_{k+1} \times d_{k+1}} \mathbf{x}_{k+2}$$

  where each $\mathbf{x}_k$ is used to compute its corresponding $g_k \equiv \nabla(\mathbf{x}_k)$
- starting in the first step, given arbitrary point $\mathbf{x}_0$:

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{x}_0 + \alpha_0 d_0 \\ g_0 &= Q\mathbf{x}_0 - b \end{aligned}$$

- obviously, we hope $\mathbf{x}_1$ to minimize the **line** (direction) $\mathbf{x}_0 + \alpha_0 d_0$
- this is equivalently saying, $g_1 \equiv \nabla f(\mathbf{x}_1) \perp (\mathbf{x}_0 + \alpha_0 d_0)$
- think this way, we now have changed the coordinates from one ortho-normal basis to another: $[x_1, x_2] \to [u, v]$ let:

$$(u = (\mathbf{x}_0 + \alpha_0 d_0) \quad \text{and} \quad v \perp u) \implies \left[\frac{\partial f}{\partial u}, \frac{\partial f}{\partial v}\right] = \left[0, \frac{\partial f}{\partial v}\right]$$

Looking at the algorithm closely

- we have,

$$
\begin{aligned}
g_1 &= \nabla f(\mathbf{x}_1) = Q\mathbf{x}_1 - b \\
&= Q(\mathbf{x}_0 + \alpha_0 d_0) - b = (Q\mathbf{x}_0 - b) + \alpha_0 Q d_0 \\
&= g_0 + \alpha_0 Q d_0
\end{aligned}
$$

- $g_1 \not\perp d_0$ in general, but we can show a particular choice α_0 makes it do, i.e., x_1 minimizes the line $\mathbf{x}_0 + \alpha_0 d_0$

$$
\begin{aligned}
d_0^\top g_1 &= d_0^\top g_0 + d_0^\top \alpha_0 Q d_0 && \times d_0^\top \text{ on each side} \\
&= d_0^\top g_0 + \alpha_0 d_0^\top Q d_0 \\
&= d_0^\top g_0 - \frac{d_0^\top g_0}{d_0^\top Q d_0} d_0^\top Q d_0 && \text{sub } \alpha_0 = -\frac{d_0^\top g_0}{d_0^\top Q d_0} \\
&= d_0^\top g_0 - d_0^\top g_0 = 0 \\
\implies & d_0 \perp g_1
\end{aligned}
$$

- above shows the choice d_0 is also somewhat arbitrary
- **to understand** by choose a different $\mathbf{x}_0$, results a different g_0, having an arbitrary (g_0, d_0) pair results a unique $\alpha_0 = -\frac{d_0^\top g_0}{d_0^\top Q d_0}$ making $\mathbf{x}_1$ the minimum of the **line** $\mathbf{x}_0 + \alpha_0 d_0$
- however, a sensible choice is $d_0 = -\nabla f(\mathbf{x}_0) = -g_0$

Expanding Subspace Theorem

- knowing $g_1 \perp d_0$, we also can prove similarly that:

$$g_k \perp \text{span}(\underbrace{d_0, \ldots, d_{k-1}}_{k \text{ terms}})$$

for example, if $\mathbf{x}_2 \perp (\mathbf{x}_0 + \alpha_0 d_0)$ and $\mathbf{x}_2 \perp (\mathbf{x}_1 + \alpha_1 d_1)$, we know that $\mathbf{x}_2 \perp$ a **surface** span of the two perpendicular lines d_0 and d_1, we write this as:

$$g_2 \perp \text{span}(\underbrace{d_0, d_1}_{2 \text{ terms}})$$

we can drop $\mathbf{x}_0$ and $\mathbf{x}_1$

- we can see that $\mathbf{x}_k$ minimizes f over $\left\{\mathbf{x}_0 + \text{span}(d_0, \ldots, d_{k-1})\right\}$
- therefore, it's obvious"

$$\mathbf{x}_n = \underset{\mathbf{x} \in \{\mathbf{x}_0 + \text{span}(d_0, \ldots, d_{n-1})\}}{\arg\min} \frac{1}{2}\mathbf{x}^\top Q\mathbf{x} - b^\top \mathbf{x}$$

determine directions

- one more thing missing, we know it works well for any arbitrary Q-conjugate vectors $\{d_0, \dots, d_n\}$:
- a sensible guess of d_1 *wouldbe* (we already used $d_0 = -\nabla f(\mathbf{x}_0) = -g_0$:

$$d_1 = -\nabla f(\mathbf{x}_1) + \beta_0 d_0 = -g_1 + \beta_0 d_0$$

- use definition of conjugacy:

$$\begin{aligned} d_1^\top Q d_0 &= 0 \\ \implies (-g_1 + \beta_0 d_0)^\top d_0 &= 0 \\ -g_1^\top Q d_0 + \beta_0 d_0^\top Q d_0 &= 0 \\ \beta_0 &= \frac{g_1^\top Q d_0}{d_0{}^\top Q d_0} \end{aligned}$$

Conjugate Gradient Algorithm

1. let f be a quadratic function:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top Q\mathbf{x} + b^\top \mathbf{x} + c$$

2. **initialize**: Let $i = 0$ and $\mathbf{x}_i = \mathbf{x}_0$, $d_i = d_0 = \nabla f(\mathbf{x}_0)$
3. compute α_0 to minimize the function $f(\mathbf{x}_i + \alpha d_i)$:

$$\begin{aligned}\alpha_k &= -\frac{{d_k}^\top(Q\mathbf{x}_k + b)}{{d_k}^\top Q d_k} \\ &= -\frac{d_k^\top g_k}{d_k^\top Q d_k}\end{aligned}$$

4. update

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha d_k$$

5. update the direction:

$$\beta_k = \frac{g_{k+1}^\top Q d_k}{{d_k}^\top Q d_k}$$

6. Repeat steps 2-4 until we have looked in n directions, where $\mathbf{x} \in \mathbb{R}^n$

A quick demo to show Stochastic Gradient Descent (1)

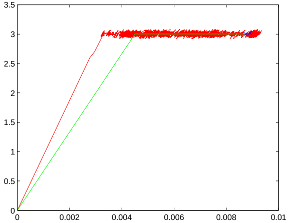
A simple example:

$$F(\theta) = \|\mathbf{x}^T\theta - \mathbf{y}\|^2 = \sum_{i=1}^{N} \left(x_i^T\theta - y_i\right)^2$$

$$\begin{aligned}\nabla F(\theta) &= 2\mathbf{x}^T(\mathbf{x}\theta - \mathbf{y}) \\ &\propto \mathbf{x}\theta - \mathbf{y} \\ &= \sum_{i=1}^{N} x_i^T\theta - y_i\end{aligned}$$

- Traditional gradient descent approach: $\theta_{n+1} = \theta_n - \alpha_n \left(\sum_{i=1}^{N} x_i^T\theta - y_i\right)$
- However, think about what if N is $1,000,000$, which happens often in the BIG DATA era.
- Stochastic Gradient Descent HELPS!

A quick demo to illustrate Stochastic Gradient Descent (2)



Idea, instead of

$$\theta_{n+1} = \theta_n - \alpha_n \left(\sum_{i=1}^{N} x_i^T \theta - y_i \right)$$

Each iteration, we select randomly a data point pair (x_j, y_j), and do:

$$\theta_{n+1} = \theta_n - \alpha_n \left(x_j^T \theta - y_j \right) \qquad j \sim U(1, \dots N)$$

It surprisingly works quite well in many settings. See demo

q-norm Regulariser

- The objective function:

$$E_D(\mathbf{w}) + \alpha E_W(\mathbf{w})$$

- Example:

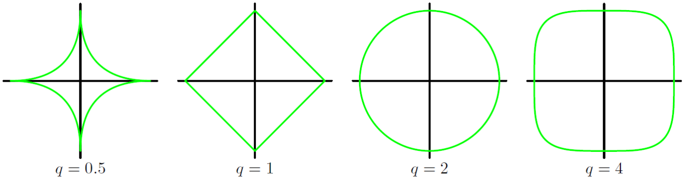
$$\frac{1}{2}\sum_{n=1}^{N}\Big(t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\Big)^2 + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} \implies \mathbf{w}_{\text{ML}} = \Big(\alpha\mathbf{I} + \mathbf{\Phi}^T\mathbf{\Phi}\Big)^{-1}\mathbf{\Phi}^T\mathbf{t}$$

- A generalised example:

$$\frac{1}{2}\sum_{n=1}^{N}\Big(t_n - \mathbf{w}^T\phi(\mathbf{x}_n)\Big)^2 + \frac{\alpha}{2}\sum_{j=1}^{M}|w_j|^q \implies \mathbf{w}_{\text{ML}} \text{ not so easy to obtain}$$

Diagrams of ϕ_j and struggle between $E_D(\mathbf{w})$ and $\alpha E_W(\mathbf{w})$

Plot of various norm functions: q-norm $\|\mathbf{w}\|_q := \left(\sum_{i=1}^n |w_i|^q \right)^{1/q} = 1$:



minimise $E_D(\mathbf{w}) + \alpha E_W(\mathbf{w})$ becomes the "tradeoff" between the two: