Gradient descent

Summary

A classical problem of function minimization is considered.

$$x_{k+1} = x_k - \eta_k \nabla f(x_k) \tag{GD}$$

- The bottleneck (for almost all gradient methods) is choosing step-size, which can lead to the dramatic difference in method's behavior.
- One of the theoretical suggestions: choosing stepsize inversly proportional to the gradient Lipschitz constant $\eta_k = \dfrac{1}{L}$.
- In huge-scale applications the cost of iteration is usually defined by the cost of gradient calculation (at least $\mathcal{O}(p)$).
- If function has Lipschitz-continious gradient, then method could be rewritten as follows:

$$\begin{aligned} x_{k+1} &= x_k - \frac{1}{L}\nabla f\left(x_k\right) = \\ &= \arg\min_{x \in \mathbb{R}^n} \left\{ f\left(x_k\right) + \langle \nabla f\left(x_k\right), x - x_k \rangle + \frac{L}{2}\|x - x_k\|_2^2 \right\} \end{aligned}$$

Intuition

Direction of local steepest descent

Let's consider a linear approximation of the differentiable function f along some direction $h, \|h\|_2 = 1$:

$$f(x + \eta h) = f(x) + \eta \langle f'(x), h \rangle + o(\eta)$$

We want h to be a decreasing direction:

$$f(x + \eta h) < f(x)$$

$$f(x) + \eta \langle f'(x), h \rangle + o(\eta) < f(x)$$

and going to the limit at $\eta \to 0$:

$$\langle f'(x), h \rangle \leq 0$$

Also from Cauchy–Bunyakovsky–Schwarz inequality:

$$|\langle f'(x), h \rangle| \leq \|f'(x)\|_2 \|h\|_2 \quad \to \quad \langle f'(x), h \rangle \geq -\|f'(x)\|_2 \|h\|_2 = -\|f'(x)\|_2$$

Thus, the direction of the antigradient

$$h = -\frac{f'(x)}{\|f'(x)\|_2}$$

gives the direction of the **steepest local** decreasing of the function f.

The result of this method is

$$x_{k+1} = x_k - \eta f'(x_k)$$

Gradient flow ODE

Let's consider the following ODE, which is referred as Gradient Flow equation.

$$\frac{dx}{dt} = -f'(x(t))$$

and discretize it on a uniform grid with η step:

$$\frac{x_{k+1} - x_k}{\eta} = -f'(x_k),$$

where $x_k \equiv x(t_k)$ and $\eta = t_{k+1} - t_k$ - is the grid step.

From here we get the expression for x_{k+1}

$$x_{k+1} = x_k - \eta f'(x_k),$$

which is exactly gradient descent.

Necessary local minimum condition

$$\begin{aligned}
&f'(x) = 0 \\
&-\eta f'(x) = 0 \\
&x - \eta f'(x) = x \\
&x_k - \eta f'(x_k) = x_{k+1}
\end{aligned}$$

This is, surely, not a proof at all, but some kind of intuitive explanation.

Minimizer of Lipschitz parabola

Some general highlights about Lipschitz properties are needed for explanation. If a function $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable and its gradient satisfies Lipschitz conditions with constant L, then $\forall x, y \in \mathbb{R}^n$:

$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| \leq \frac{L}{2} \|y - x\|^2,$$

which geometrically means, that if we'll fix some point $x_0 \in \mathbb{R}^n$ and define two parabolas:

$$\phi_1(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle - \frac{L}{2} \|x - x_0\|^2,$$

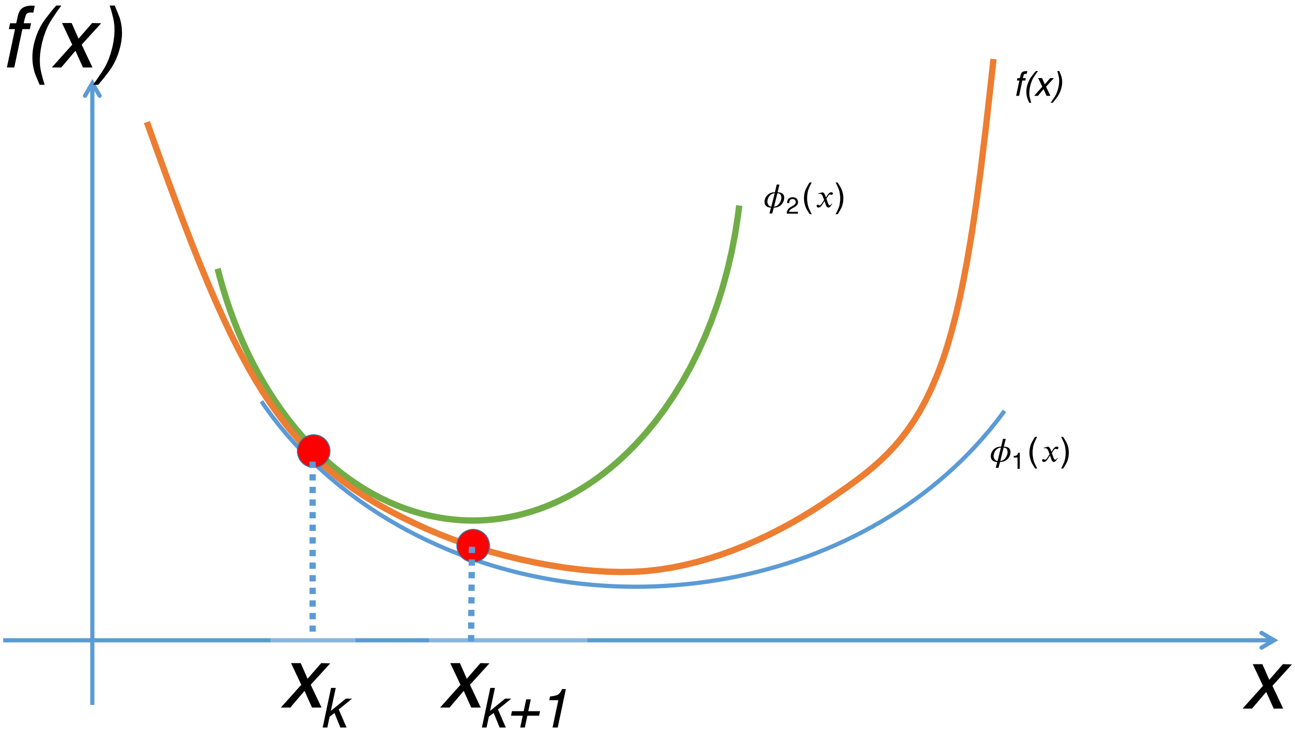
$$\phi_2(x) = f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{L}{2} \|x - x_0\|^2.$$

Then

$$\phi_1(x) \leq f(x) \leq \phi_2(x) \quad \forall x \in \mathbb{R}^n.$$

Now, if we have global upper bound on the function, in a form of parabola, we can try to go directly to its minimum.

$$
\begin{aligned}
&\nabla \phi_2(x) = 0 \\
&\nabla f(x_0) + L(x^* - x_0) = 0 \\
&x^* = x_0 - \frac{1}{L}\nabla f(x_0) \\
&x_{k+1} = x_k - \frac{1}{L}\nabla f(x_k)
\end{aligned}
$$



This way leads to the $\frac{1}{L}$ stepsize choosing. However, often the L constant is not known.

But if the function is twice continuously differentiable and its gradient has Lipschitz constant L, we can derive a way to estimate this constant $\forall x \in \mathbb{R}^n$:

$$\|\nabla^2 f(x)\| \leq L$$

or

$$-LI_n \preceq \nabla^2 f(x) \preceq LI_n$$

Stepsize choosing strategies

Stepsize choosing strategy η_k significantly affects convergence. General {%include link.html title='Line search algorithms might help in choosing scalar parameter.

Constant stepsize

For $f \in C_L^{1,1}$:

$$\eta_k = \eta$$

$$f(x_k) - f(x_{k+1}) \geq \eta \left(1 - \frac{1}{2}L\eta\right)\|\nabla f(x_k)\|^2$$

With choosing $\eta = \frac{1}{L}$, we have:

$$f(x_k) - f(x_{k+1}) \geq \frac{1}{2L} \|\nabla f(x_k)\|^2$$

Fixed sequence

$$\eta_k = \frac{1}{\sqrt{k+1}}$$

The latter 2 strategies are the simplest in terms of implementation and analytical analysis. It is clear that this approach does not often work very well in practice (the function geometry is not known in advance).

Exact line search aka steepest descent

$$\eta_k = \arg\min_{\eta \in \mathbb{R}^+} f(x_{k+1}) = \arg\min_{\eta \in \mathbb{R}^+} f(x_k - \eta \nabla f(x_k))$$

More theoretical than practical approach. It also allows you to analyze the convergence, but often exact line search can be difficult if the function calculation takes too long or costs a lot.

Interesting theoretical property of this method is that each following iteration is orthogonal to the previous one:

$$\eta_k = \arg\min_{\eta \in \mathbb{R}^+} f(x_k - \eta \nabla f(x_k))$$

Optimality conditions:

$$\nabla f(x_{k+1})^\top \nabla f(x_k) = 0$$

Goldstein-Armijo

Convergence analysis

Convex case

Lipischitz continuity of the gradient

Assume that $f: \mathbb{R}^n \to \mathbb{R}$ is convex and differentiable, and additionally

$$\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\| \; \forall x, y \in \mathbb{R}^n$$

i.e. , ∇f is Lipschitz continuous with constant $L > 0$.

Since ∇f Lipschitz with constant L, which means $\nabla^2 f \preceq LI$, we have $\forall x, y, z$:

$$(x - y)^\top (\nabla^2 f(z) - LI)(x - y) \leq 0$$

$$(x - y)^\top \nabla^2 f(z)(x - y) \leq L \|x - y\|^2$$

Now we'll consider second order Taylor approximation of $f(y)$ and Taylor’s Remainder Theorem (we assum, that the function f is continuously differentiable), we have $\forall x, y, \exists z \in [x, y]$:

$$
\begin{aligned}
f(y) &= f(x) + \nabla f(x)^\top (y-x) + \frac{1}{2}(x-y)^\top \nabla^2 f(z)(x-y) \\
&\leq f(x) + \nabla f(x)^\top (y-x) + \frac{L}{2}\|x-y\|^2
\end{aligned}
$$

For the gradient descent we have $x = x_k, y = x_{k+1}, x_{k+1} = x_k - \eta_k \nabla f(x_k)$:

$$
\begin{aligned}
f(x_{k+1}) &\leq f(x_k) + \nabla f(x_k)^\top (-\eta_k \nabla f(x_k)) + \frac{L}{2}(\eta_k \nabla f(x_k))^2 \\
&\leq f(x_k) - \left(1 - \frac{L\eta}{2}\right)\eta \|\nabla f(x_k)\|^2
\end{aligned}
$$

Optimal constant stepsize

Now, if we'll consider constant stepsize strategy and will maximize $\left(1 - \frac{L\eta}{2}\right)\eta \to \max\limits_\eta$, we'll get $\eta = \frac{1}{L}$.

$$
f(x_{k+1}) \leq f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2
$$

Convexity

$$
f(x_k) \leq f(x^*) + \nabla f(x_k)^\top (x_k - x^*)
$$

That's why we have:

$$
\begin{aligned}
f(x_{k+1}) &\leq f(x^*) + \nabla f(x_k)^\top (x_k - x^*) - \frac{1}{2L}\|\nabla f(x_k)\|^2 \\
&= f(x^*) + \frac{L}{2}\left(\|x_k - x^*\|^2 - \|x_k - x^* - \frac{1}{L}\nabla f(x_k)\|^2\right) \\
&= f(x^*) + \frac{L}{2}\left(\|x_k - x^*\|^2 - \|x_{k+1} - x^*\|^2\right)
\end{aligned}
$$

Thus, summing over all iterations, we have:

$$
\begin{aligned}
\sum_{i=1}^k (f(x_i) - f(x^*)) &\leq \frac{L}{2}\left(\|x_0 - x^*\|^2 - \|x_k - x^*\|^2\right) \\
&\leq \frac{L}{2}\|x_0 - x^*\|^2 = \frac{LR^2}{2},
\end{aligned}
$$

where $R = \|x_0 - x^*\|$. And due to convexity:

$$
f(x_k) - f(x^*) \leq \frac{1}{k}\sum_{i=1}^k (f(x_i) - f(x^*)) \leq \frac{LR^2}{2k} = \frac{R^2}{2\eta k}
$$

Strongly convex case

If the function is strongly convex:

$$
f(y) \geq f(x) + \nabla f(x)^\top (y-x) + \frac{\mu}{2}\|y-x\|^2 \; \forall x, y \in \mathbb{R}^n
$$

...

$$\|x_{k+1} - x^*\|^2 \leq (1 - \eta\mu)\|x_k - x^*\|^2$$

Bounds

Conditions	$\|f(x_k) - f(x^*)\| \leq$	**Type of convergence**	$\|x_k - x^*\| \leq$
Convex Lipschitz-continuous function(G)	$\mathcal{O}\left(\dfrac{1}{k}\right) \; \dfrac{GR}{k}$	Sublinear	
Convex Lipschitz-continuous gradient (L)	$\mathcal{O}\left(\dfrac{1}{k}\right) \; \dfrac{LR^2}{k}$	Sublinear	
μ-Strongly convex Lipschitz-continuous gradient(L)		Linear	$(1 - \eta\mu)^k R^2$
μ-Strongly convex Lipschitz-continuous hessian(M)		Locally linear $R < \overline{R}$	$\dfrac{\overline{R}R}{\overline{R} - R}\left(1 - \dfrac{2\mu}{L + 3\mu}\right)$

- $R = \|x_0 - x^*\|$ - initial distance
- $\overline{R} = \dfrac{2\mu}{M}$

Materials

- The zen of gradient descent. Moritz Hardt
- Great visualization
- Cheatsheet on the different convergence theorems proofs

Inexact line search

This strategy of inexact line search works well in practice, as well as it has the following geometric interpretation:

Sufficient decrease

Let's consider the following scalar function while being at a specific point of x_k:

$$\phi(\alpha) = f(x_k - \alpha\nabla f(x_k)), \alpha \geq 0$$

consider first order approximation of $\phi(\alpha)$:

$$\phi(\alpha) \approx f(x_k) - \alpha\nabla f(x_k)^\top \nabla f(x_k)$$

A popular inexact line search condition stipulates that α should first of all give sufficient decrease in the objective function f, as measured by the following inequality:

$$f(x_k - \alpha\nabla f(x_k)) \leq f(x_k) - c_1 \cdot \alpha\nabla f(x_k)^\top \nabla f(x_k)$$

for some constant $c_1 \in (0, 1)$. (Note, that $c_1 = 1$ stands for the first order Taylor approximation of $\phi(\alpha)$). This is also called Armijo condition. The problem of this condition is, that it could accept arbitrary small values α, which may slow down solution of the problem. In practice, c_1 is chosen to be quite small, say $c_1 \approx 10^{-4}$.

Curvature condition

To rule out unacceptably short steps one can introduce a second requirement:

$$-\nabla f(x_k - \alpha\nabla f(x_k))^\top \nabla f(x_k) \geq c_2 \nabla f(x_k)^\top(-\nabla f(x_k))$$

for some constant $c_2 \in (c_1, 1)$, where c_1 is a constant from Armijo condition. Note that the left-handside is simply the derivative $\nabla_\alpha \phi(\alpha)$, so the curvature condition ensures that the slope of $\phi(\alpha)$ at the target point is greater than c_2 times the initial slope $\nabla_\alpha \phi(\alpha)(0)$. Typical values of $c_2 \approx 0.9$ for Newton or quasi-Newton method. The sufficient decrease and curvature conditions are known collectively as the Wolfe conditions.

Goldstein conditions

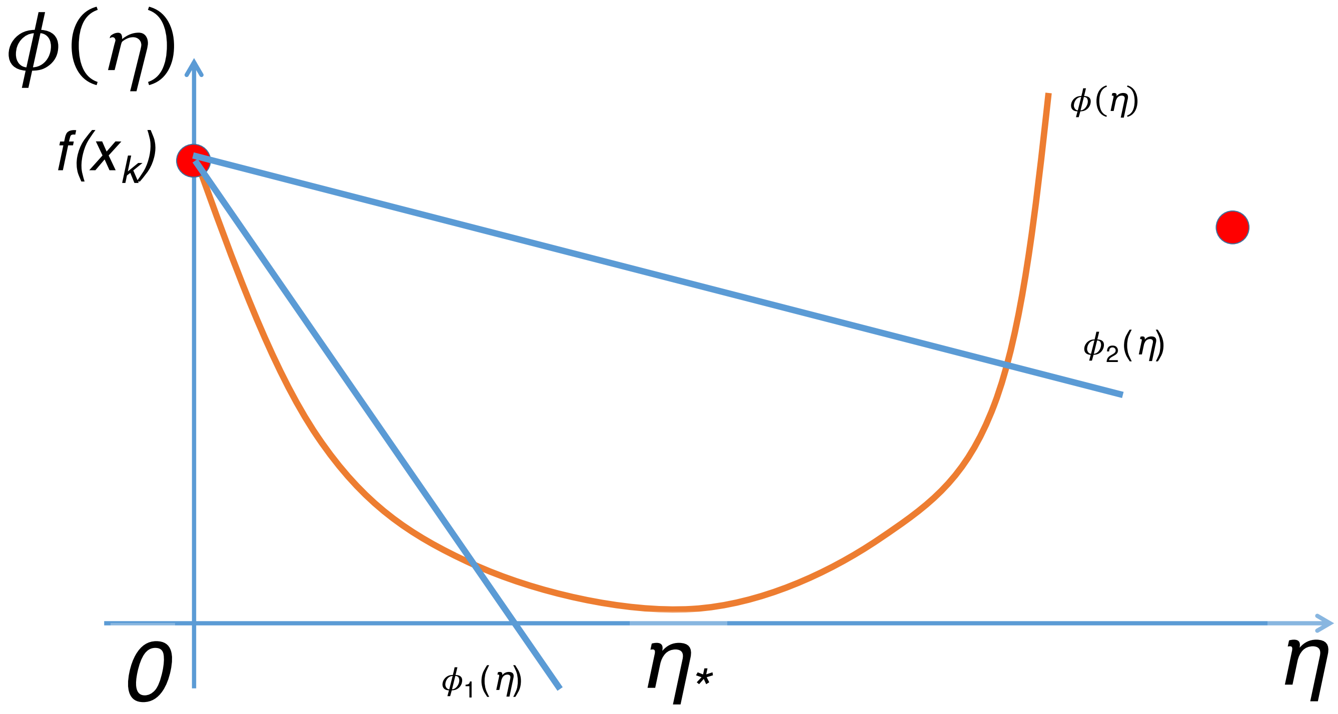
Let's consider also 2 linear scalar functions $\phi_1(\alpha), \phi_2(\alpha)$:

$$\phi_1(\alpha) = f(x_k) - \alpha\alpha\|\nabla f(x_k)\|^2$$

and

$$\phi_2(\alpha) = f(x_k) - \beta\alpha\|\nabla f(x_k)\|^2$$

Note, that Goldstein-Armijo conditions determine the location of the function $\phi(\alpha)$ between $\phi_1(\alpha)$ and $\phi_2(\alpha)$. Typically, we choose $\alpha = \rho$ and $\beta = 1 - \rho$, while $\rho \in (0.5, 1)$.



References

- Numerical Optimization by J.Nocedal and S.J.Wright.