Line Search Methods Analysis

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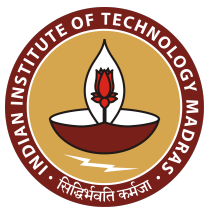

Step Length

- In computing the step length we face a trade-off.
- We want to choose α_k to give a substantial reduction of f, but we don't want to spend too much time making the choice.
- Off-course the ideal choice would be the global minimiser of the univariate function $\phi(.)$ defined by

$$\phi(\alpha) = f(x_k + \alpha p_k), \ \alpha > 0. \tag{1}$$

- But in general, it is too expensive to identify this value.
- It requires too many evaluations of the objective function and/or the gradient to even find a local minimiser to moderate precision.

Step Length

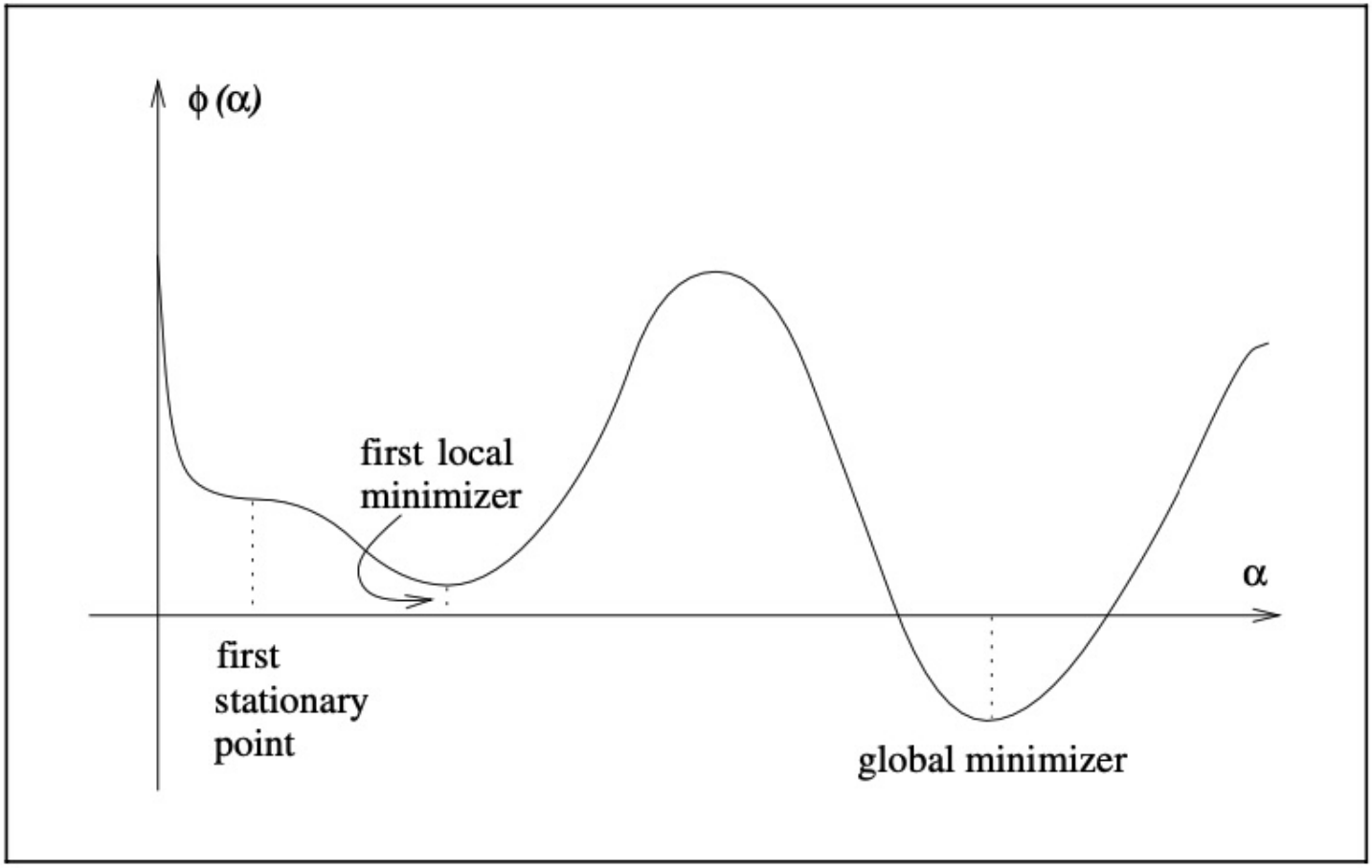

Figure: The ideal step length is the global minimiser

Step Length

- Practically, strategies perform an inexact line search to identify a step length that achieves adequate reductions in f at minimal cost.
- We will discuss these search strategies a little later.
- We will now discuss various termination conditions for line search algorithms and show that effective step lengths need not lie near minimisers of the univariate function $\phi(\alpha)$.
- Is $f(x_k + \alpha_k p_k) < f(x_k)$ good enough to get convergence??
- for example consider the function

$$f(x) = x^2 - 1$$

it has the global minima at $x = 0$, $f = -1$.

Step Length

- Consider a sequence $\{x_k\}$ s.t.

$$f(x_k) = \frac{5}{k}, \quad k = 1, 2, 3, \ldots$$
$$\implies f(x_k) > f(x_{k+1})$$

- The reduction in f at each step is not enough to get it to converge to the minimiser.

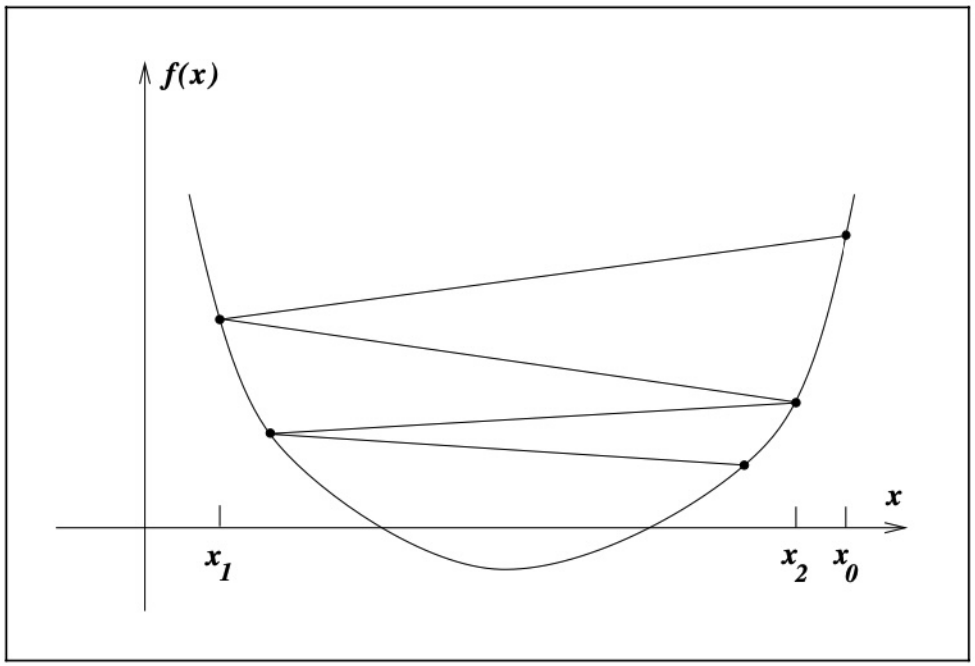

Figure: Insufficient reduction

The Wolfe Condition

Armijo Condition (Sufficient Decrease Condition):

α_k should be chosen such that

$$f(x_k + \alpha p_k) \leq f(x_k) + c_1 \alpha \nabla f_k^T p_k \tag{2}$$

for some constant $c_1 \in (0, 1)$.

- Since p_k is a descent direction and $c_1 > 0$ and $\alpha > 0$ the first thing that the Armijo condition asserts that there is a reduction in f from x_k to $x_{k+1} = x_k + \alpha p_k$.
- The reduction in f is atleast

$$c_1 \alpha \nabla f_k^T p_k$$

therefore it also says the reduction in f must be proportional to both the step length α_k and the directional derivative $\nabla f_k^T p_k$

The Wolfe Condition

- The right hand side of (2) is a linear function in α (say) $l(\alpha)$.

$$l(\alpha) = f(x_\alpha) + c_1 \alpha \nabla f_k^T p_k$$

- The function $l(.)$ has a negative slope $c_1 \nabla f_k^T p_k$ but $c_1 \in (0, 1)$.
- Therefore, it lies above the graph of ϕ for small positive values of α.
- The sufficient decrease condition states that α is acceptable only if

$$\phi(\alpha) \leq l(\alpha).$$

- In practice, c_1 is chosen to be quite small, say

$$c_1 = 10^{-4}$$

The Wolfe Condition

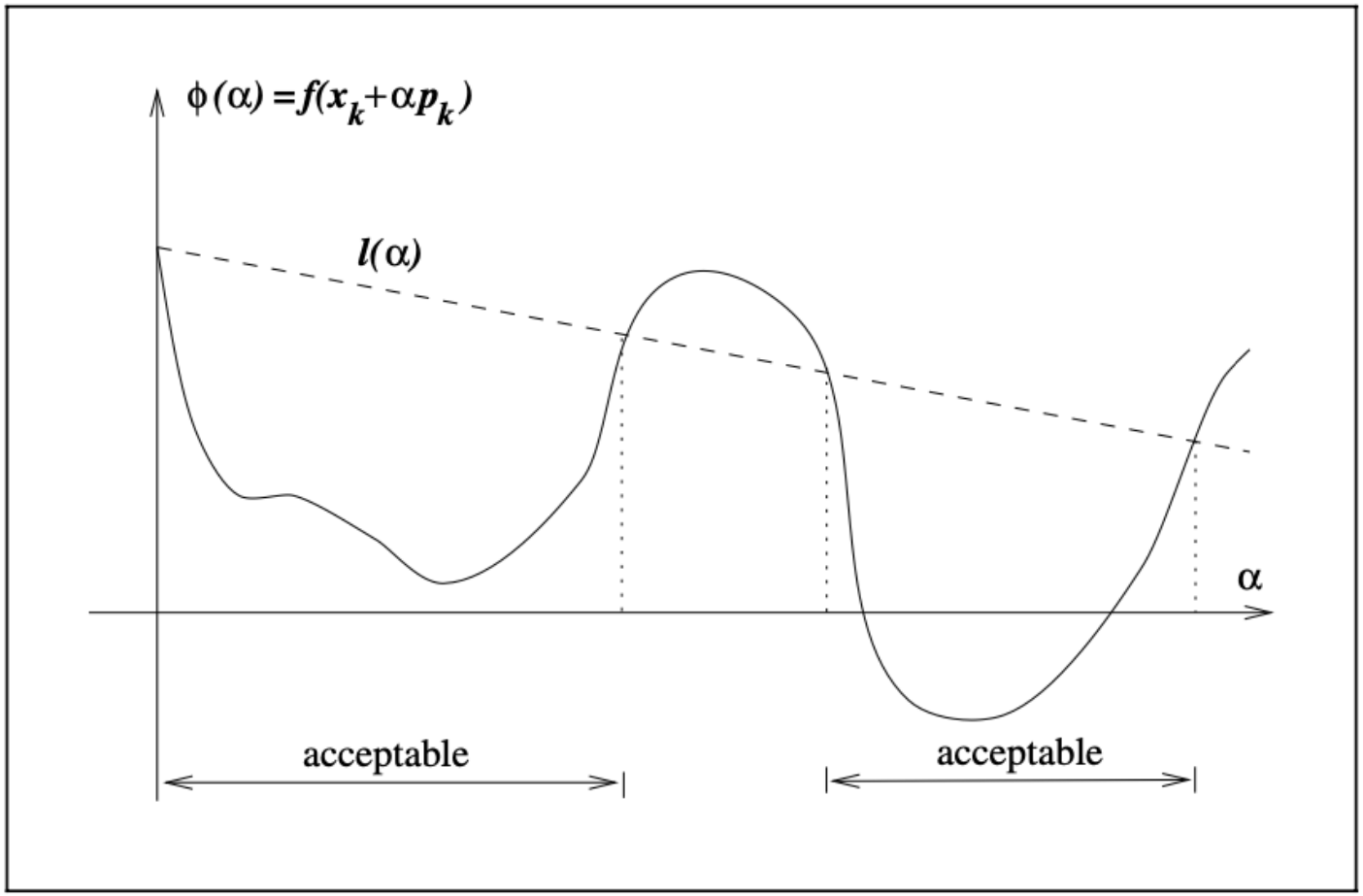

Figure: The intervals on which the Armijo condition is satisfied is shown

The Wolfe Condition

- The sufficient decrease condition is not enough by itself to ensure that the algorithm makes reasonable progress.
- As it is satisfied for all sufficiently small values of α

The Wolfe Condition

- To rule out unacceptable short steps we introduce a second requirement.

Curvature Conditions

α_k should satisfy

$$\nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f_k^T p_k \tag{3}$$

for some constant $c_2 \in (c_1, 1)$.

- The left-hand side is simply the derivative $\phi'(\alpha_k)$.
- So the curvature condition ensures that the slope of ϕ at α_k is greater than c_2 times the initial slope $\phi'(0)$.
- If the slope $\phi'(\alpha)$ is strongly negative, we have an indication that we can reduce f significantly by moving further along the chosen direction.

The Wolfe Condition

- On, the other hand if $\phi'(\alpha)$ is only slightly negative or even positive, it is a sign that we cannot expect much more decrease in f in this direction.
- So it makes sense to terminate the line search. (See Figure 6)
- Typical values of c_2 are 0.9 when the search direction p_k is chosen by a Newton or quasi-Newton method, and 0.1 when p_k is obtained from a non-linear conjugate gradient method.
- The sufficient decrease and curvature conditions are known collectively as the Wolfe conditions.

The Wolfe Condition

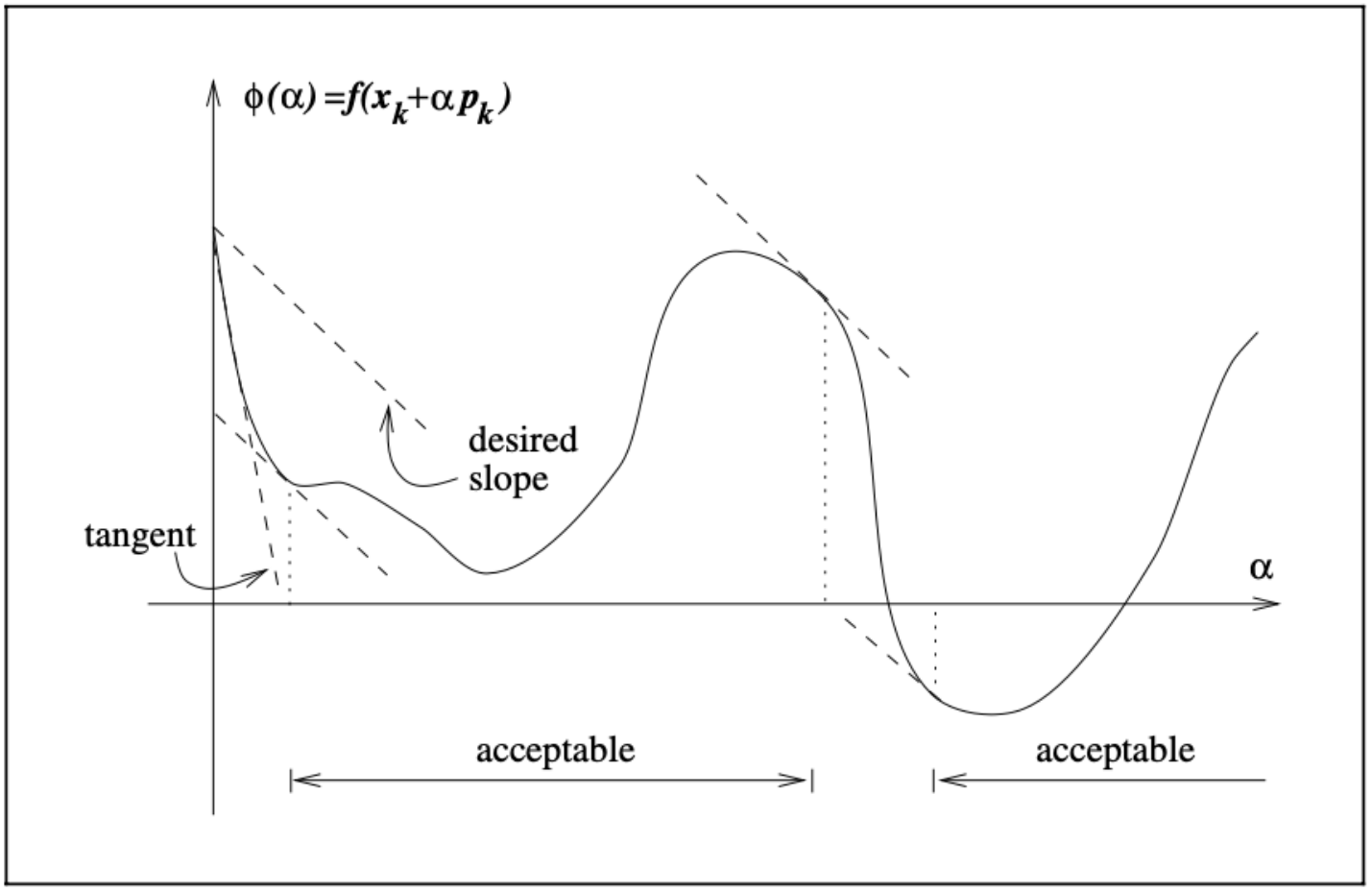

Figure: Insufficient Reduction

Wolfe Conditions

$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k \nabla f_k^T p_k$$
$$\nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f_k^T p_k. \tag{4}$$

with $0 < c_1 < c_2 < 1$.

- A step length may satisfy the Wolfe conditions without being particularly close to a minimiser of ϕ. (See previous figure)
- The curvature conditions can be modified to force α_k to lie in atleast a broad neighbourhood of a local minimiser or stationary point of ϕ.

The Strong Wolfe Conditions

α_k is required to satisfy

$$f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k \nabla f_k^T p_k$$
$$|\nabla f(x_k + \alpha_k p_k)^T p_k| \leq c_2 |\nabla f_k^T p_k|. \tag{5}$$

with $0 < c_1 < c_2 < 1$.

- The only difference with the Wolfe conditions is that we no longer allow the derivative $\phi'(\alpha)$ to be too positive.
- It excludes points that are far from stationary points of ϕ.
- Is it always possible to find step lengths that satisfy Wolfe conditions ?

The Wolfe Condition

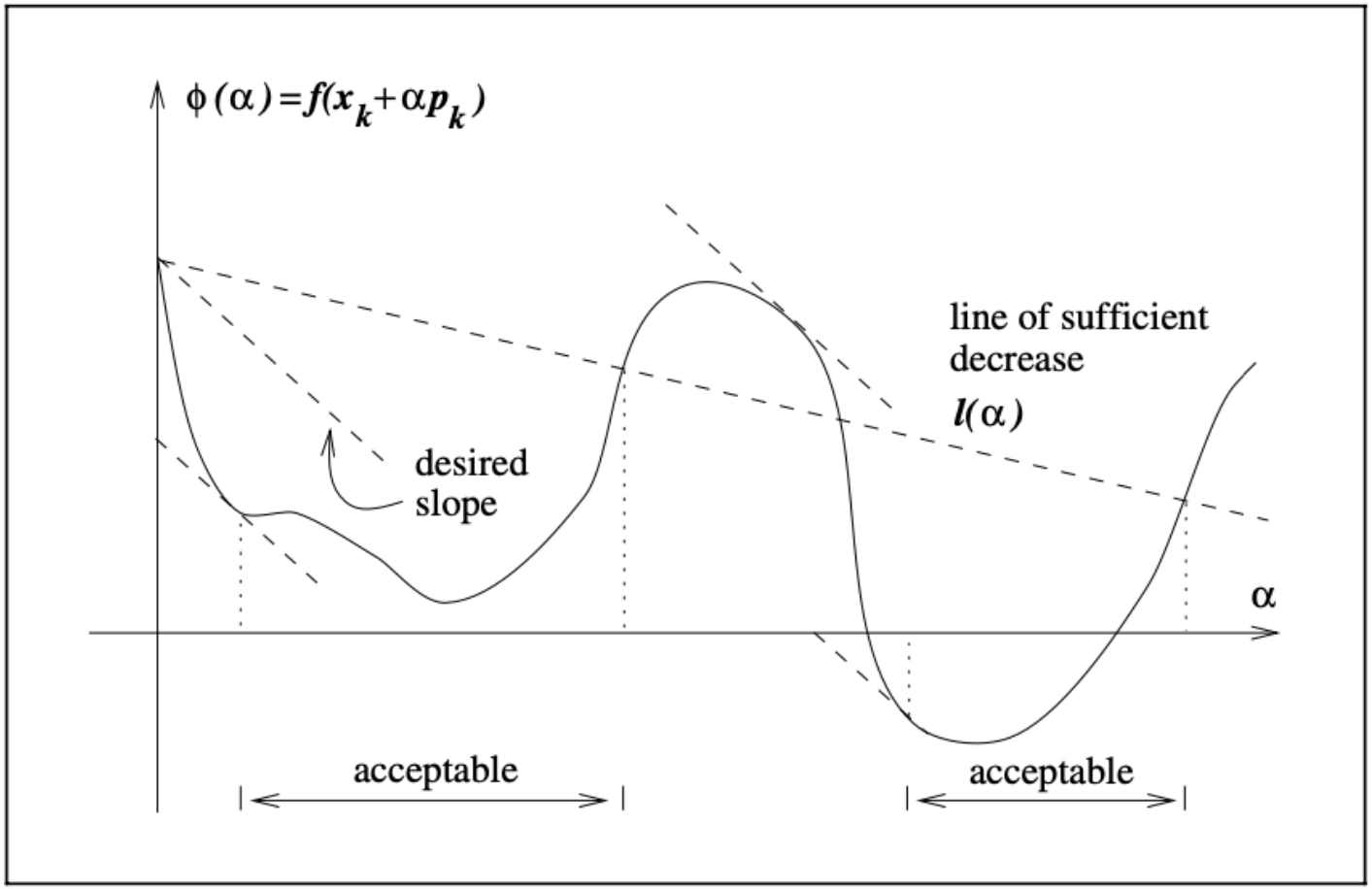

Figure: Step Lengths satisfying the Wolfe conditions.

Existence of α satisfying Wolfe conditions

Lemma

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable. Let p_k be a descent direction at x_k, and assume that f is bounded below along the ray

$$\{x_k + \alpha p_k \mid \alpha > 0\}$$

Then if $0 < c_1 < c_2 < 1$, there exist intervals of step lengths satisfying Wolfe conditions and the strong Wolfe conditions.

Sketch of Proof

- $$\phi(\alpha) = f(x_k + \alpha p_k)$$

  is bounded below for all $\alpha > 0$
- Let $l(\alpha) = f(x_k) + \alpha c_1 \nabla f_k^T p_k$, the line is unbounded below and must intersect the graph of ϕ atleast once.

Existence of α satisfying Wolfe conditions

- Note that for very small values if α (we can find such α)

$$\begin{aligned} l(\alpha) &= f(x_k) + \alpha c_1 \nabla f_k^T p_k \\ &> f(x_k) + \alpha \nabla f_k^T p_k \qquad \text{as } \nabla f_k^T p_k < 0 \text{ and } c_1 < 1 \\ &\approx f(x_k + \alpha p_k) = \phi(\alpha). \end{aligned}$$

  Therefore, to start with, the graph of $l(\alpha)$ stays above $\phi(\alpha)$.
- Now since $\phi(\alpha)$ is bounded below $\exists$ a minimum value and since $l(\alpha)$ is unbounded below it will (for large values of α) attain values lesser than the minimum value of $\phi(\alpha)$. Therefore, both the graphs will intersect atleast once.
- Let $\alpha' > 0$ be the smallest intersecting value of α that is

$$f(x_k + \alpha' p_k) = f(x_k) + \alpha' c_1 \nabla f_k^T p_k.$$

Existence of α satisfying Wolfe conditions

- α' is the point where the line $l(\alpha)$ meets $\phi(\alpha)$ for the first time . Therefore for all $\alpha < \alpha'$ the sufficient decrease condition holds good.
- Now by applying the mean value theorem on $\phi(\alpha)$ in the interval $[0, \alpha']$ we get

$$\frac{\phi(\alpha') - \phi(0)}{\alpha' - 0} = \phi'(\alpha'') \qquad \alpha'' \in (0, \alpha')$$
$$\implies f(x_k + \alpha' p_k) - f(x_k) = \alpha' \nabla f(x_k + \alpha'' p_k)^T p_k$$
$$\implies f(x_k + \alpha' p_k) = f(x_k) + \alpha' \nabla f(x_k + \alpha'' p_k)^T p_k$$

$$\nabla f(x_k + \alpha'' p_k)^T p_k = c_1 \nabla f_k^T p_k > c_2 \nabla f_k^T p_k \qquad (6)$$
$$\text{since } c_2 > c_1 \text{and } \nabla f_k^T p_k < 0.$$

- α'' satisfies the Wolfe conditions and the inequalities hold strictly for both the condition.

Existence of α satisfying Wolfe conditions

- Hence, by our smoothness assumption on f, there is an interval around α'' for which the Wolfe conditions hold.
- Moreover, since the left-hand side term in the curvature condition is negative, the strong Wolfe condition also holds in the same interval.

The Goldstein Conditions

The Goldstein are stated as a pair of inequalities, in the following way:

$$f(x_k)+(1-c)\alpha_k \nabla f_k^T p_k \leq f(x_k+\alpha_k p_k) \leq f(x_k)+c\alpha_k \nabla f_k^T p_k, \quad (7)$$

with $0 < c < \frac{1}{2}$.

- The second inequality is the sufficient decrease condition.
- Whereas the first inequality is introduced to control the step length from below.
- A disadvantage of the Goldstein conditions vis-a-vis the Wolfe conditions is that the first inequality in (7) may exclude all minimizers of ϕ.
- However, the Goldstein and Wolfe conditions have much in common, and their convergence theories are quite similar.

The Goldstein Conditions

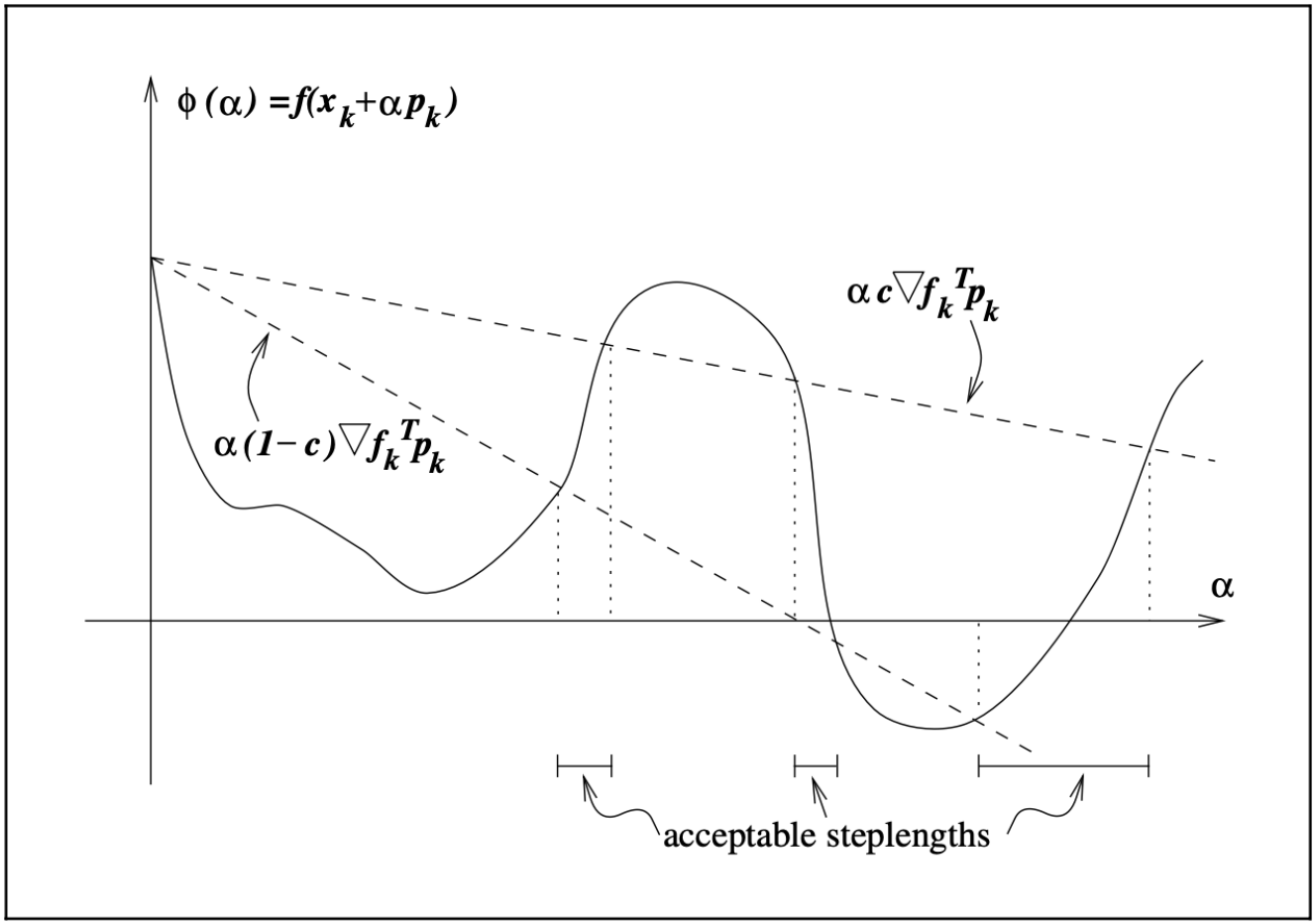

Figure: The Goldstein conditions.

Sufficient Decrease and Backtracking

- The sufficient decrease condition alone is not sufficient to ensure that the algorithm makes reasonable progress along the given search direction.
- However, the extra curvature condition can be dispensed off by using a so-called backtracking approach to choose candidate step length.

Backtracking Line Search

1. Choose $\bar{\alpha} > 0$, $\rho \in (0,1)$, $c \in (0,1)$;
2. Set $\alpha = \bar{\alpha}$
3. While $f(x_k + \alpha p_k) > f(x_k) + c\alpha \nabla f_K^T p_k$
4. $\alpha = \rho\alpha$;
5. end.

Terminate with $\alpha_k = \alpha$.

Sufficient Decrease and Backtracking

- The initial step length $\bar{\alpha}$ is chosen to be 1 in Newton and quasi-Newton methods, but can have different values in other algorithms, such as steepest descent or conjugate gradient.
- An acceptable step length will be found in a finite number of steps as α_k will eventually become small enough to satisfy the sufficient decrease condition.
- In practice the contraction factor "ρ" is allowed to vary at each iteration of the line search.
- One may need to ensure that $\rho \in [\rho_{lo}, \rho_{hi}]$ for some fixed constants $0 < \rho_{lo} < \rho_{hi} < 1$.

Sufficient Decrease and Backtracking

- The backtracking approach either choose $\alpha_k = \bar{\alpha}$ the initial choice or else α_k is short enough to satisfy the sufficient decrease condition.
- Still α_k is not very small as, $\frac{\alpha_k}{\rho}$ doesn't satisfy the sufficient decrease condition.
- It is only by a factor of $\frac{1}{\rho}$ that α_k is shorter from the previous choice of α_k which doesn't work.
- It is a very simple and quite a popular strategy to terminate line search algorithms.
- Well suited for Newton methods but less appropriate for quasi-Newton and conjugate gradient methods.

Convergence of Line Search Methods

Global Convergence

$$||\nabla f_k|| \to 0 \qquad \text{as } k \to \infty$$

i.e. convergence to a stationary point for any starting point x_0.

To obtain global convergence:

1. Need to choose step lengths well;
2. Choose search directions p_k appropriately as well.
   - Let p_k be a chosen direction at the kth iteration of the line search method.
   - We define θ_k to be the angle between p_k and the steepest descent direction $-\nabla f_k$ given by

$$\cos\theta = \frac{-\nabla f_k^T p_k}{||\nabla f_k||\ ||p_k||} \tag{8}$$

Global Convergence

Theorem (Zountendijk)

Consider any iteration of the form

$$x_{k+1} = x_k + \alpha_k p_k$$

where p_k is a descent direction and α_k satisfies the Wolfe conditions. Suppose that f is bounded below in $\mathbb{R}^n$ and that f is continuously differentiable in an open set $\mathcal{N}$ containing the level set

$$\mathcal{L} =^{def} \{x : f(x) \leq f(x_0)\}$$

where x_0 is the starting point of the iteration. Assume also that the gradient "∇f" is Lipschitz continuous on $\mathcal{N}$, i.e. there exists a constant $L > 0$ s.t.

$$||\nabla f(x) - \nabla f(\tilde{x})|| \leq L||x - \tilde{x}||, \qquad \text{for all } \; x, \tilde{x} \in \mathcal{N}$$

Then

$$\sum_{k \geq 0} \cos^2 \theta_k ||\nabla f_k||^2 < \infty$$

Global Convergence

Proof:

- Consider the second Wolfe condition,

$$\begin{aligned} & \nabla f(x_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f_k^T p_k \\ \text{or, } & \nabla f(x_{k+1})^T p_k \geq c_2 \nabla f_k^T p_k \\ \text{or, } & \nabla f(x_{k+1})^T p_k - \nabla f(x_k)^T p_k \geq (c_2 - 1) \nabla f_k^T p_k \\ \text{or, } & (\nabla f(x_{k+1})^T - \nabla f(x_k))^T p_k \geq (c_2 - 1) \nabla f_k^T p_k \end{aligned} \tag{9}$$

- For every descent direction, iteration lives in the level set.
- From the Lipschitz condition we have:

$$(\nabla f(x_{k+1}) - \nabla f(x_k))^T p_k \leq \alpha_k L ||p_k||^2.$$

Global Convergence

- By combining the two relation i.e. the last equation in (9) and the one above we obtain

$$\alpha_k \geq \frac{(c_2 - 1)}{L} \frac{\nabla f_k^T p_k}{||p_k||^2} \tag{10}$$

- Now consider the first Wolfe condition

$$\begin{aligned} & f(x_k + \alpha_k p_k) \leq f(x_k) + c_1 \alpha_k \nabla f_k^T p_k \\ \text{or, } & f_{k+1} \leq f_k + c_1 \alpha_k \nabla f_k^T p_k \quad (\text{ as } \nabla f_k^T p_k < 0) \\ \text{or, } & f_{k+1} \leq f_k + c_1 \frac{(c_2 - 1)}{L} \frac{(\nabla f_k^T p_k)^2}{||p_k||^2} \quad \text{using (10)} \end{aligned} \tag{11}$$

- Note that

$$\cos\theta_k = \frac{-\nabla f_k^T p_k}{||\nabla f_k||\ ||p_k||} \implies \cos^2\theta_k ||\nabla f_k||^2 = \frac{(\nabla f_k^T p_k)^2}{||p_k||^2} \tag{12}$$

Global Convergence

- Therefore, $f_{k+1} \leq f_k - \frac{c_1(1-c_2)}{L} \cos^2 \theta_k ||\nabla f_k||^2$
- Let $c = \frac{c_1(1-c_2)}{L}$.
- By summing this expression over all indices less than or equal to k, we obtain:

$$f_{k+1} \leq f_0 - c \sum_{j=0}^{k} \cos^2 \theta_j ||\nabla f_j||^2$$

- Since f is bounded below, we have $f_0 - f_{k+1}$ is less than some positive constant, for all k.
- Therefore, by taking limits in the above we obtain

$$\sum_{k=0}^{\infty} \cos^2 \theta_k \ ||\nabla f_k||^2 < \infty.$$

which concludes the proof.

Global Convergence

- Similar results also hold for the Goldstein conditions or the strong Wolfe conditions.
- For all these strategies, the step length selection implies the inequality

$$\sum_{k \geq 0} \cos^2 \theta_k \ ||\nabla f_k||^2 < \infty$$

  which is called the Zoutendijk condition.
- The assumptions of the theorem are not too restrictive.
- f needs to be bounded below for the optimisation problem to be well defined.
- The smoothness assumption - Lipschitz continuity of the gradient - is implied by many of the smoothness conditions that are used in local convergence theorems and are often satisfied in practice.

Global Convergence

- The Zoutendijk's condition implies that

$$\cos^2 \theta_k \ ||\nabla f_k||^2 \to 0$$

- If the choice of the search direction p_k is made so that it ensures that the angle θ_k is bounded away from 90°, then there is a positive constant δ s.t.

$$\cos \theta_k > \delta > 0, \qquad \text{for all } k.$$

- It now follows immediately that

$$\lim_{k \to \infty} \ ||\nabla f_k|| = 0$$

- In other words the gradient norm $||\nabla f_k|| \to 0$, provided that the search directions are never too close to orthogonality with the gradient.

Global Convergence

- Line Search + Steepest descent (for which the search direction p_k is parallel to the negative gradient) + Wolfe or Goldstein conditions $\Longrightarrow$ Produces a gradient that converges to zero.
- For line search methods the Zoutendijk condition is the strongest global convergence result that can be obtained.
- It cannot be guaranteed that the method converges to a minimiser (let alone global minimiser).
- Only insight we get is the algorithm, is attracted to stationary points.

However, by making additional requirements on the search direction p_k
-> by introducing negative curvature information from the Hessian $\nabla^2 f(x_k)$
we can strengthen these results to include convergence to a local minimiser.

Convergence for Newton-Like Methods

- Consider a Newton-like method and assume that the matrices B_k are positive definite with a uniformly bounded condition number.
- That is, there is a constant M such that

$$||B_k||\ ||B_k^{-1}|| \leq M, \quad \text{for all } k.$$