AI505

Optimization

Local Descent

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Outline

Preface

For multivariate functions, we have argued that:

- derivatives can have exponential growth in the resulting analytical expression
- calculating zeros might be challenging

Hence, minimizing by solving $\nabla f(\boldsymbol{x}) = 0$ may be computationally demanding.

Outline

Descent Direction Iteration

Descent Direction Methods use a local model to incrementally improve design point until some convergence criteria is met.

1. Check termination conditions at $\boldsymbol{x}_k$; if not met, continue.
2. Decide **descent direction** $\boldsymbol{d}_k$ using local information, commonly required that $\boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) < 0$.
3. Decide **step size** (ie, magnitude of the overall step that depends on α_k, sometimes but not always $\|\boldsymbol{d}_k\|_2 = 1$)
4. Compute next design point $\boldsymbol{x}_{k+1}$

$$\boxed{\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k}$$

Descent Direction

The search direction often has the form

$$\boldsymbol{d}_k = -B_k^{-1} \nabla f(\boldsymbol{x}_k)$$

where B_k is a symmetric and nonsingular matrix.

- in the steepest descent method, B_k is the identity matrix I
- in Newton's method, B_k is the exact Hessian $\nabla^2 f(\boldsymbol{x}_k)$.
- in quasi-Newton methods, B_k is an approximation to the Hessian that is updated at every iteration by means of a low-rank formula.

When $\boldsymbol{d}_k = -B_k^{-1} \nabla f(\boldsymbol{x}_k)$ and B_k is positive definite, we have

$$\boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) = -\nabla f(\boldsymbol{x}_k)^T B_k^{-1} \nabla f(\boldsymbol{x}_k) < 0$$

and therefore $\boldsymbol{d}_k$ is a descent direction. In fact, it is a double implication!

Outline

- We discuss how to choose α_k and $\boldsymbol{d}_k$ to promote convergence from remote starting points.
- We also consider the rate of convergence of steepest descent, quasi-Newton, and Newton methods.

Line Search for Step Size

Assuming we have the search direction:

- Use it to compute α
- Using the techniques discussed in the previous class, find the minimum of a univariate function:

$$\phi(\alpha) = f(\boldsymbol{x} + \alpha \boldsymbol{d}) \qquad \text{minimize}_{\alpha \geq 0}\ \phi(\alpha)$$

We assume that $\boldsymbol{p}_k$ is a descent direction, that is, $\phi'(0) < 0$, so that our search can be confined to positive values of α.

```
def line_search(f, x, d)
  objective = lambda alpha: f(x + alpha * d)
  a, b = bracket_minimum(objective)
  alpha = minimize(objective, a, b)
  return x + alpha * d
```

Often computationally costly, so approximate line search is used instead

Line Search: Alternatives

α is called to the **learning rate** or **step factor**:

Equal to the **step size** only when $\|\boldsymbol{d}_k\|_2 = 1$.

- Fixed learning rate
- **Decaying step factor**

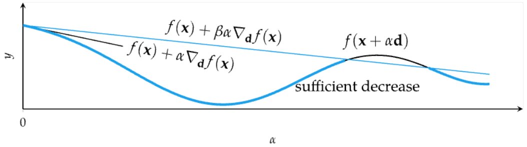
$$\alpha_k = \alpha_1 \gamma^{k-1} \qquad \text{for } \gamma \in [0, 1]$$

Decaying step factor is often required in convergence proofs

Approximate Line Search

- If function calls are expensive, rather than finding the minimum along a search direction, find a point of sufficient decrease

$$f(\boldsymbol{x}_{k+1}) \leq f(\boldsymbol{x}_k) + \beta\alpha\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)$$

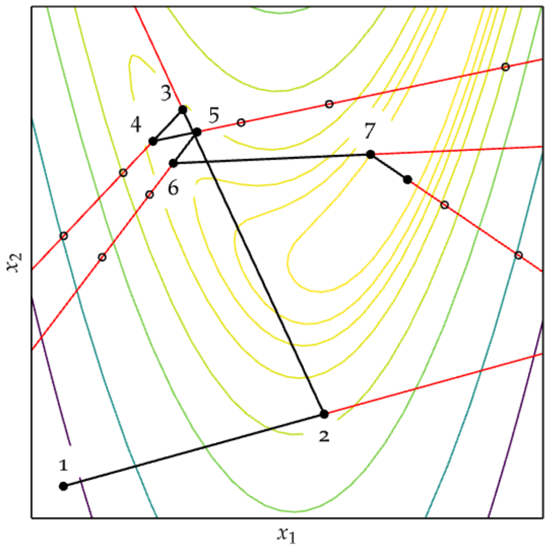


- $\beta \in [0, 1]$, usually $\beta = 1 \times 10^{-4}$
- Alone this condition is insufficient to guarantee convergence to a local minimum. It can converge prematurely.
- Backtracking line search starts with a large step and then backs off

```
def backtracking_line_search(f, grad, x, d, alpha_0=1, p=0.5, beta=1e-4):
    y, g, alpha = f(x), grad(x), alpha_0
    while ( f(x + alpha * d) > y + beta * alpha * np.dot(g, d) ) :
        alpha *= p
    return alpha
```

- Guaranteed to converge to a local minimum, but can be slow.

Approximate Line Search: Example



Approximate Line Search

Building on backtracking line search are the **Wolfe Conditions** together sufficient to guarantee convergence to a local minimum.

1. First Wolfe Condition: Sufficient Decrease (Armijo condition)

$$f(\boldsymbol{x}_{k+1}) \leq f(\boldsymbol{x}_k) + \beta\alpha\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)$$

2. Second Wolfe Condition: Curvature Condition

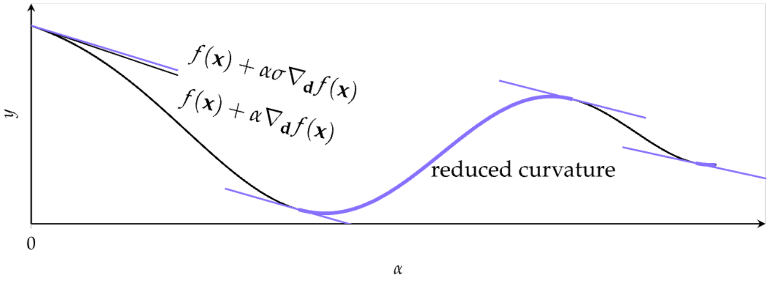
$$\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_{k+1}) \geq \sigma\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)$$

$\beta < \sigma < 1$ with
- $\sigma = 0.1$ with conjugate gradient method
- $\sigma = 0.9$ with Newton method

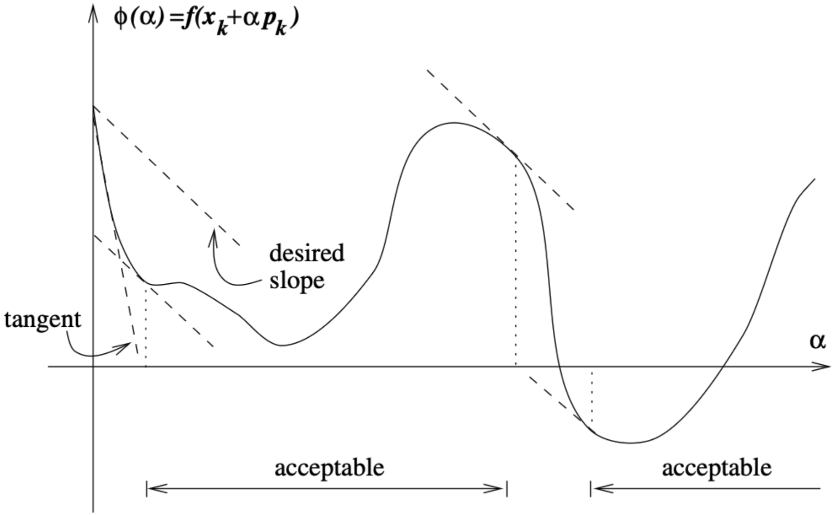
Curvature Condition

Regions satisfying the curvature condition $\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_{k+1}) \geq \sigma \nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)$

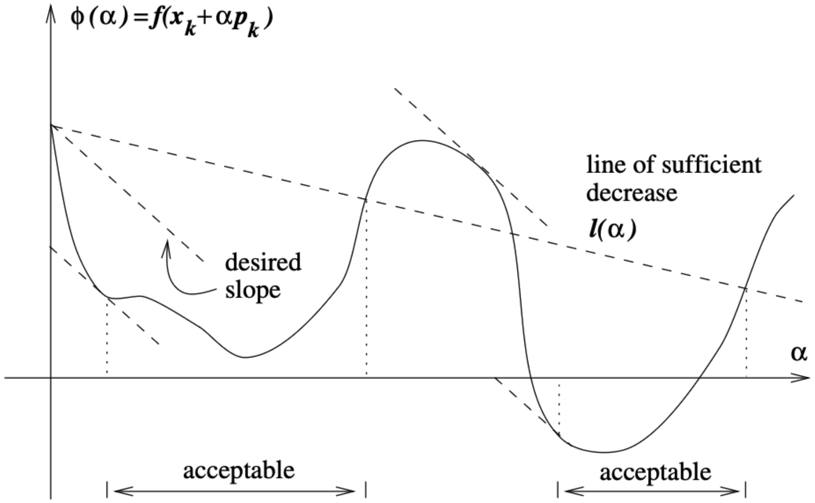
- Consider the univariate function $\phi(\alpha) = f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)$.
- The left-hand-side is simply the derivative $\phi'(\alpha_k)$, so the curvature condition ensures that the slope of ϕ at α_k is greater than σ times the initial slope $\phi'(0)$.
- If the slope $\phi'(0)$ is negative, then we are looking for a step size α_k such that the slope of ϕ at that point is still negative but not too negative.
- If $\phi'(\alpha_k)$ 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.


$f(\mathbf{x}) + \alpha\sigma\nabla_{\mathbf{d}} f(\mathbf{x})$
$f(\mathbf{x}) + \alpha\nabla_{\mathbf{d}} f(\mathbf{x})$
reduced curvature
y
0
α

Curvature Condition



Wolfe Conditions



Approximate Line Search: Example

Consider approximate line search on $f(x_1, x_2) = x_1^2 + x_1 x_2 + x_2^2$
from $\boldsymbol{x} = [1, 2]$ in the direction $\boldsymbol{d} = [-1, -1]$, gradient at $\boldsymbol{x}$ is $\boldsymbol{g} = [4, 5]$
using a maximum step size of 10, a reduction factor of 0.5,
first Wolfe condition parameter $\beta = 1 \times 10^{-4}$, second Wolfe condition parameter $\sigma = 0.9$.

First Wolfe condition $(f(\boldsymbol{x} + \alpha \boldsymbol{d}) \leq f(\boldsymbol{x}) + \beta\alpha(\boldsymbol{g}^T \cdot \boldsymbol{d}))$:

$$\begin{aligned}
\alpha = 10: &\quad f([1,2] + 10 \cdot [-1,-1]) \leq 7 + 1 \times 10^{-4} 10 [4,5]^T [-1,-1] \implies 217 \not\leq 6.991 \\
\alpha = 10 \cdot 0.5 = 5: &\quad f([1,2] + 5 \cdot [-1,-1]) \leq 7 + 1 \times 10^{-4} 5 [4,5]^T [-1,-1] \implies 37 \not\leq 6.996 \\
\alpha = 2.5: &\quad f([1,2] + 2.5 \cdot [-1,-1]) \leq 7 + 1 \times 10^{-4} 2.5 [4,5]^T [-1,-1] \implies 3.25 \leq 6.998
\end{aligned}$$

The candidate design point $\boldsymbol{x}' = \boldsymbol{x} + \alpha \boldsymbol{d} = [-1.5, -.0.5]$ is checked against the second Wolfe condition $\nabla_{\boldsymbol{d}} f(\boldsymbol{x}') \geq \sigma \nabla_{\boldsymbol{d}} f(\boldsymbol{x})$:

$$[-3.5, -2.5] \cdot [-1, -1] \geq \sigma [4, 5] \cdot [-1, -1] \implies 6 \geq -8.1$$

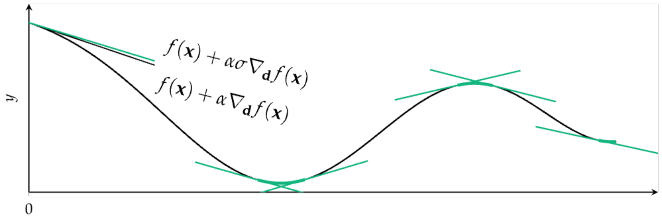
Approximate line search terminates with $\boldsymbol{x} = [-1.5, -0.5]$.

Strong Wolfe Conditions

A step length may satisfy the Wolfe conditions without being particularly close to a minimizer of $f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)$.
We can modify the curvature condition to force $f(\boldsymbol{x}_{k+1})$ to exclude points that are far from stationary points of $f(\boldsymbol{x}_{k+1})$, ie, we no longer allow the gradient $\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_{k+1})$ to be too positive.

Strong Wolf conditions:

$$f(\boldsymbol{x}_{k+1}) \leq f(\boldsymbol{x}_k) + \beta\alpha\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k) \qquad \text{and} \qquad |\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_{k+1})| \leq \sigma |\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)|$$



Approximate Line Search Goal

Given:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$$

with descent direction:

$$\nabla f(\boldsymbol{x}_k)^T \boldsymbol{d}_k < 0$$

Define:

$$\phi(\alpha) = f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k), \qquad \phi'(\alpha) = \nabla f(\boldsymbol{x}_k + \alpha \boldsymbol{d}_k)^T \boldsymbol{d}_k$$

Goal:

Find $\alpha > 0$ satisfying the **Strong Wolfe Conditions**.

Strong Wolfe Conditions

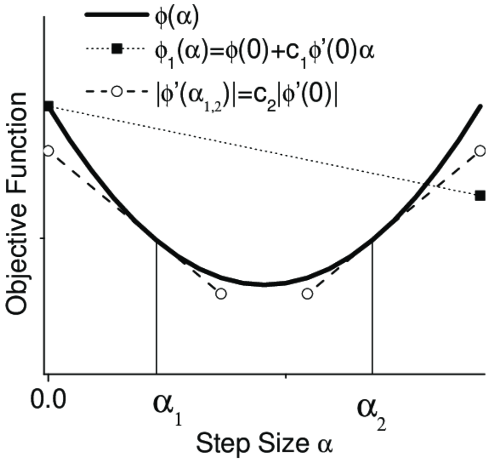
Two requirements:

Sufficient decrease (Armijo)

$$\phi(\alpha) \leq \phi(0) + \beta\alpha\phi'(0)$$

Strong curvature condition

$$|\phi'(\alpha)| \leq \sigma|\phi'(0)|$$



Ensures:

- sufficient decrease
- step near minimum

Strong Backtracking: Idea

Two phases:

1. Bracketing phase

- Start with $[\alpha_0 = 0, \alpha_1 = 1]$
- Increase step
- Find interval containing solution

2. Zoom phase

- Shrink interval
- Use bisection or interpolation
- Find Wolfe step

Idea:

Bracket minimum $\rightarrow$ **Zoom to solution**

Algorithm

Bracketing

- Start with $[\alpha_0 = 0, \alpha_{max} = 1]$
- If Armijo fails or slope changes sign

  $\rightarrow$ Zoom

- If strong Wolfe satisfied

  $\rightarrow$ Stop

- Else increase step

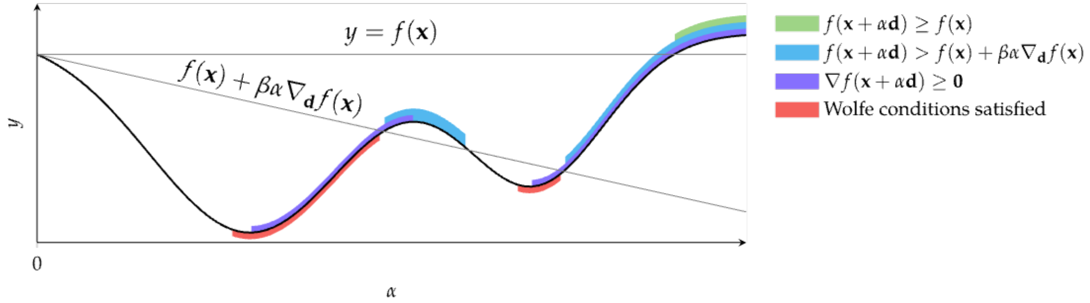
```
Input   : $\alpha_{max}$
Output: $\alpha^*$ set to a step length that satisfies the
        strong Wolfe condition
Initialize $k \leftarrow 0$;
Set $\alpha_0 \leftarrow 0$, choose $\alpha_{max} > 0$ and $\alpha_1 \in (0, \alpha_{max})$;
$i \leftarrow 1$;
while True do
    Evaluate $\phi(\alpha_i)$;
    if $\phi(\alpha_i) > \phi(0) + \beta\alpha_i\phi'(0)$ or
     $[\phi(\alpha_i) \geq \phi(\alpha_i - 1)$ and $i > 1]$ then
        $\alpha^* \leftarrow \text{zoom}(\alpha_{i-1}, \alpha_i)$ and break;
    Evaluate $\phi'(\alpha_i)$;
    if $|\phi'(\alpha_i)| \leq -\sigma\phi'(0)$ then
        set $\alpha^* \leftarrow \alpha_i$ and break;
    if $\phi'(\alpha_i) \geq 0$ then
        set $\alpha^* \leftarrow \text{zoom}(\alpha_i, \alpha_{i-1})$ and break;
    Choose $\alpha_i + 1 \in (\alpha_i, \alpha_{max})$; // Eg, $\alpha_{i+1} \leftarrow 2\alpha_i$
    $i \leftarrow i + 1$;
```

Bracketing Phase

begins with a trial estimate α_1, and keeps increasing it until it finds either an acceptable step length or an interval that brackets the desired step lengths guaranteed to satisfy the strong Wolfe conditions

The interval (α_{i-1}, α_i) contains step lengths satisfying the strong Wolfe conditions if one of the following three conditions is satisfied:

1. $\phi(\alpha_i) > \phi(0) + \beta\alpha_i\phi'(0)$ (ie, α_i violates the sufficient decrease condition);
2. $\phi(\alpha_i) \geq \phi(\alpha_{i-1})$;
3. $\phi'(\alpha_i) \geq 0$.



Algorithm

Zoom

- Interpolate inside bracket
- Shrink interval
- Stop when Wolfe satisfied

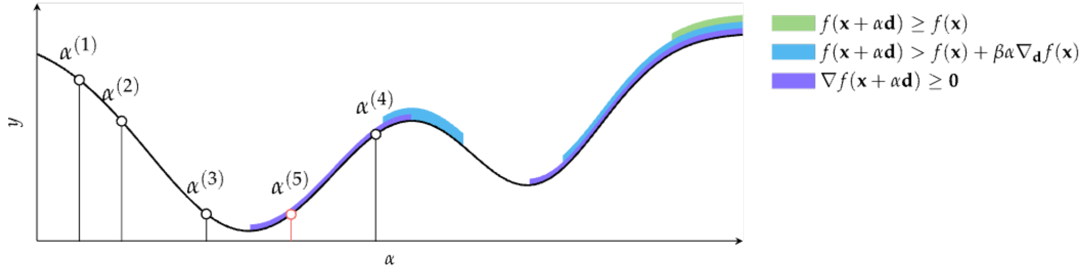
Iterate generating an $\alpha_j \in [\alpha_{lo}, \alpha_{hi}]$, and then replacing one of these endpoints by α_j such that:

1. $[\alpha_{lo}, \alpha_{hi}]$ satisfy the strong Wolfe conditions;
2. α_{lo} smallest function value;
3. α_{hi} chosen so that $\phi'(\alpha_{lo})(\alpha_{hi} - \alpha_{lo}) < 0$.

```
Input   : $\alpha_{lo}, \alpha_{hi}$
Output: $\alpha^*$ set to a step length that satisfies the strong Wolfe condition
while True do
    Interpolate (using quadratic, cubic or bisection) to find a trial step
     length $\alpha_j$ between $\alpha_{lo}$ and $\alpha_{hi}$ ;
    Evaluate $\phi(\alpha_j)$;
    if $\phi(\alpha_j) > \phi(0) + \beta\alpha_j\phi'(0)$ or $\phi(\alpha_j) \geq \phi(\alpha_{lo})$ then
        $\alpha_{hi} \leftarrow \alpha_j$;
    else
        Evaluate $\phi'(\alpha_j)$;
        if $|\phi'(\alpha_j)| \leq -\sigma\phi'(0)$ then
            Set $\alpha^* \leftarrow \alpha_j$ and break;
        if $\phi'(\alpha_j)(\alpha_{hi} - \alpha_{lo}) \geq 0$ then
            $\alpha_{hi} \leftarrow \alpha_{lo}$;
        $\alpha_{lo} \leftarrow \alpha_j$;
```

Zoom phase

successively decreases the size of the interval until an acceptable step length is identified.



Approximate Line Search

```
def strong_backtracking(f, nabla, x, d; alpha=1, beta=1e-4, sigma=0.1)
  y0, g0, y_prev, alpha_prev = f(x), nabla(x) @ d, NaN, 0
  alpha_lo, alpha_hi = NaN, NaN
```

```
  # bracket phase
  while true
    y = f(x + alpha*d)
    if y > y0 + beta*alpha*g0 || (!isnan(y_prev)↪
         ↪ && y >= y_prev)
      alpha_lo, alpha_hi = alpha_prev, alpha
      break
    dir_gradient = g(x + alpha*d) @ d
    if abs(dir_gradient) <= -sigma * g0
      return alpha
    elif dir_gradient <= 0
      alpha_lo, alpha_hi = alpha, alpha_prev
      break
    y_prev, alpha_prev, alpha = y, alpha, 2 * ↪
         ↪alpha
```

```
  # zoom phase
  ylo = f(x + alpha_lo*d)
  while true:
    alpha = (alpha_lo + alpha_hi)/2
    y = f(x + alpha*d)
    if y > y0 + beta*alpha*g0 || y >= ↪
         ↪ylo
      alpha_hi = alpha
    else
      g = nabla(x + alpha*d) @ d
      if abs(g) <= -sigma*g0
        return alpha
      elif g*(alpha_hi -alpha_lo) >= 0
        alpha_hi = alpha_lo
      alpha_lo = alpha
```

Why Strong Backtracking?

Used in:

- Gradient descent
- Quai-Newton BFGS, L-BFGS
- Nonlinear Conjugate Gradient

Guarantees:

- global convergence
- stable steps
- fast convergence of quasi-Newton

Standard method in modern optimization.

Note: it is an algorithm that make use of derivative information!

Outline

Convergence Analysis

Let $\{\boldsymbol{x}_k\}$ be a sequence of points belonging in $\mathbb{R}^n$.
We say that a sequence $\{\boldsymbol{x}_k\}$ converges to some point $\boldsymbol{x}$, written $\lim_{k\text{ß}\infty} \boldsymbol{x}_k = x$, if for any $\epsilon > 0$, there is an index K such that

$$\|\boldsymbol{x}_k - \boldsymbol{x}\| \leq \epsilon \qquad \text{for all } k \geq K$$

For example, the sequence $\boldsymbol{x}_k$ defined by $\boldsymbol{x}_k = (1 - 2^{-k}, 1/k^2)^T$ converges to $(1, 0)^T$.

Convergence of Line Search

Let θ_k be the angle between $\boldsymbol{d}_k$ and the steepest descent direction $-\nabla f_k$, defined by:

$$\cos\theta_k = \frac{-\nabla f_k^T \boldsymbol{d}_k}{\|\nabla f_k\| \, \|\boldsymbol{d}_k\|}$$

Theorem (Zoutendijk condition)

Consider any iteration of the form $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$, where $\boldsymbol{d}_k$ 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 N containing the level set $\mathcal{L} = \{x : f(x) \leq f(x_0)\}$, where x_0 is the starting point of the iteration. Assume also that the gradient ∇f is Lipschitz continuous on N, that is, there exists a constant $L > 0$ such that:

$$|f(x) - f(y)| \leq L|x - y|, \quad \forall x, y \in N$$

Then:

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

The Zoutendijk condition implies that

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

We can be sure that the gradient norms $\|\nabla f_k\|$ converge to zero, provided that the search directions are never too close to orthogonality with the gradient.

It is a **global convergence** result.
Here the strongest possible result: we cannot guarantee that the method converges to a minimizer, but only that it is attracted by stationary points. (only introducing the Hessian we can prove convergence to a local minimum)

In

$$\boldsymbol{d}_k = -B_k^{-1} \nabla f(\boldsymbol{x}_k)$$

assume that the matrices B_k are **positive definite** with a uniformly bounded condition number. That is, there is a constant M such that $\|B_k\| \left\|B_k^{-1}\right\| \leq M$ for all k.

Then from the definition of θ_k:

$$\cos \theta_k \geq 1/M$$

By combining this bound with $\cos^2 \theta_k \left\|\nabla f_k\right\|^2 \to 0$ we find that

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

So, globally convergent under the positive definitness assumptions on B_k, (which is needed to ensure that $\boldsymbol{p}_k$ is a descent direction), and if the step lengths satisfy the Wolfe conditions.

Rate of Convergence

Let $\{\boldsymbol{x}_k\}$ be a sequence in $\mathbb{R}^n$ that converges to $\boldsymbol{x}^*$.
The convergence is said to be **Q-linear** (quotient-linear) if there is a constant $r \in (0, 1)$ such that

$$\boxed{\frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} \leq r \qquad \text{for all } k \text{ sufficiently large}}$$

ie, the distance to the solution $\boldsymbol{x}^*$ decreases at each iteration by at least a constant factor bounded away from 1 (ie, < 1).

Example:
sequence $\{1 + (0.5)^k\}$ converges Q-linearly to 1, with rate $r = 0.5$.

Rate of Convergence

The convergence is said to be **Q-superlinear** if

$$\boxed{\lim_{k\to\infty} \frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} = 0}$$

Example: the sequence $\{1 + k^{-k}\}$ converges superlinearly to 1.

An even more rapid convergence rate: The convergence is said to be **Q-quadratic** if

$$\boxed{\frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^2} \leq M \qquad \text{for all } k \text{ sufficiently large}}$$

where M is a positive constant, not necessarily less than 1. Example: the sequence $\{1 + (0.5)^{2^k}\}$. The values of r and M depend not only on the algorithm but also on the properties of the particular problem. Regardless of these values a quadratically convergent sequence will always eventually converge faster than a linearly convergent sequence.

Rate of Convergence

Superlinear convergence (quadratic, cubic, quartic, etc) is regarded as fast and desirable, while sublinear convergence is usually impractical.

- Steepest descent algorithms converge only at a Q-linear rate, and when the problem is ill-conditioned the convergence constant r in is close to 1.
- Quasi-Newton methods for unconstrained optimization typically converge Q-superlinearly
- Newton's method converges Q-quadratically under appropriate assumptions.

Rate of Convergence

A slightly weaker form of convergence:
overall rate of decrease in the error, rather than the decrease over each individual step of the algorithm.
We say that convergence is **R-linear** (root-linear) if there is a sequence of nonnegative scalars $\{v_k\}$ such that

$\|\boldsymbol{x}_k - \boldsymbol{x}^*\| \leq \{v_k\}$ for all k, and $\{v_k\}$ converges Q-linearly to zero.

Outline

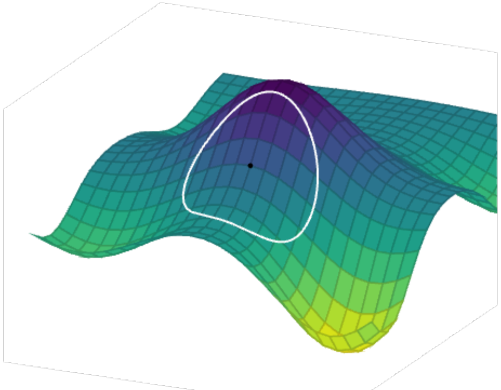
Trust Region Methods

- Descent methods can place too much trust in their first and second order information
- A **trust region** is the local area of the design space where the local model is believed to be reliable.
- Trust region methods, or restricted step methods, limit the step size to ensure local approximation error is minimized
- If the improvement matches the predicted value, the trust region is expanded; otherwise it is contracted

Trust Region Methods

- $\boldsymbol{x}'$ is new design point
- $\hat{f}(\boldsymbol{x}')$ is local function approximation, eg, second-order Taylor approximation
- δ is trust region radius

$$\begin{aligned} &\text{minimize}_{\boldsymbol{x}'} \hat{f}(\boldsymbol{x}') \\ &\text{subject to} \quad ||\boldsymbol{x} - \boldsymbol{x}'|| \leq \delta \end{aligned}$$



Constrained optimization problem.
It can be solved efficiently if $\hat{f}$ quadratic

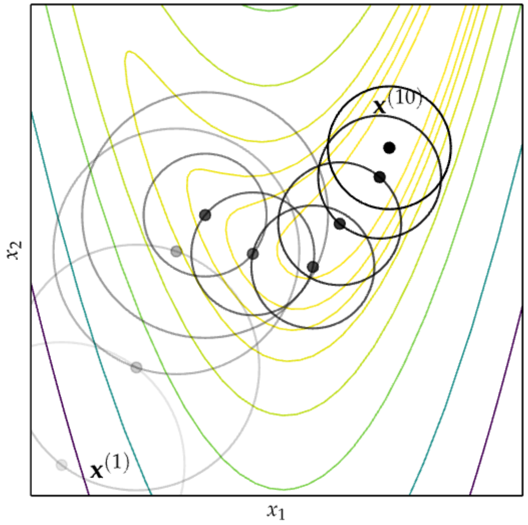
Trust Region Methods

δ can be expanded or contracted based on performance

$$\eta = \frac{\text{actual improvement}}{\text{predicted improvement}} = \frac{f(\boldsymbol{x}) - f(\boldsymbol{x}')}{f(\boldsymbol{x}) - \hat{f}(\boldsymbol{x}')}$$

If $\eta < \eta_1$ contract by a factor $\gamma_k < 1$
if $\eta > \eta_2$ expand by a factor $\gamma_k > 1$

Trust Region Methods: Example



Trust regions can be also non circular.

Trust Region Methods

Termination Conditions (commonly used together):

- Maximum Iterations: $k > k_{\max}$
- Aboslute Improvement: $f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) < \epsilon_a$
- Relative Improvement: $f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) < \epsilon_r |f(\boldsymbol{x}_k)|$
- Gradient Magnitude: $||\nabla f(\boldsymbol{x}_{k+1})|| < \epsilon_g$

Then random restart.

Summary

- Descent direction methods incrementally descend toward a local optimum.
- Univariate optimization can be applied during line search.
- Approximate line search can be used to identify appropriate descent step sizes.
- Trust region methods constrain the step to lie within a local region that expands or contracts based on predictive accuracy.
- Termination conditions for descent methods can be based on criteria such as the change in the objective function value or magnitude of the gradient.