

AI505
Optimization

Local Descent

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Outline

1. Line Search Methods
2. Convergence Analysis
3. Trust Region Methods

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 $\nabla f(\mathbf{x}) = \mathbf{0}$ may be computationally demanding.

Outline

1. Line Search Methods

2. Convergence Analysis

3. Trust Region Methods

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

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

Descent Direction

The search direction often has the form

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

where B_k is a symmetric and nonsingular matrix.

- in the steepest descent method, B_k is the identity matrix \mathbf{I}
- in Newton's method, B_k is the exact Hessian $\nabla^2 f(\mathbf{x}_k)$.
- 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 $\mathbf{d}_k = -B_k^{-1} \nabla f(\mathbf{x}_k)$ and B_k is positive definite, we have

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

and therefore \mathbf{d}_k is a descent direction.

Outline

- we discuss how to choose α_k and 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, solve:

$$\text{minimize}_{\alpha} f(\mathbf{x} + \alpha \mathbf{d})$$

```
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 $\|\text{stepsize}\|$ only when $\|\mathbf{d}_k\|_2 = 1$.

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

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

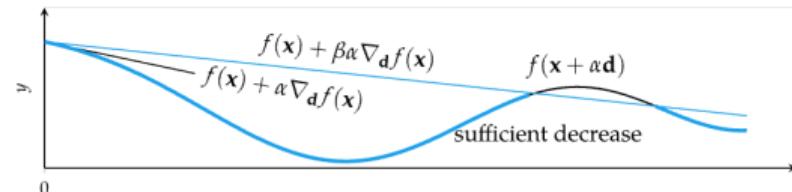
Decaying step factor is often required in convergence proofs

Approximate Line Search

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

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

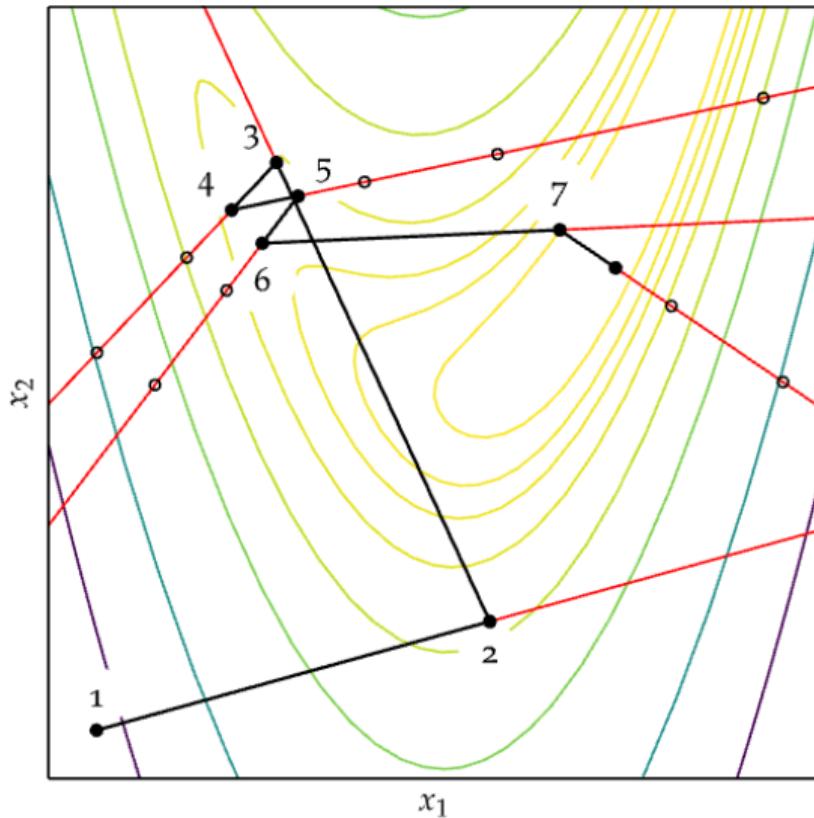
- $\beta \in [0, 1]$, usually $\beta = 1 \times 10^{-4}$
- Alone this condition is insufficient to guarantee convergence to a local minimum. It can converge prematurely.
- Backtracking line search starts with a large step and then backs off



```
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)

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

2. Second Wolfe Condition: Curvature Condition

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

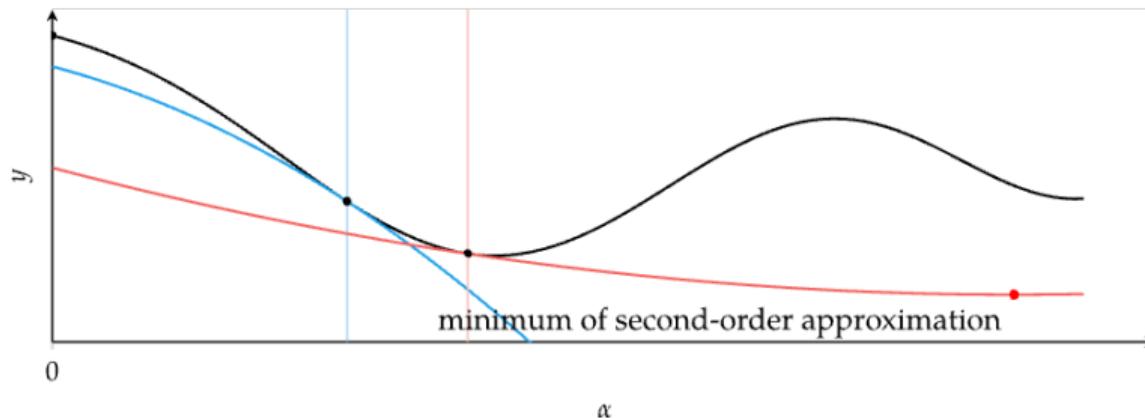
$\beta < \sigma < 1$ with

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

Approximate Line Search

The curvature condition ensures the second-order function approximations have positive curvature

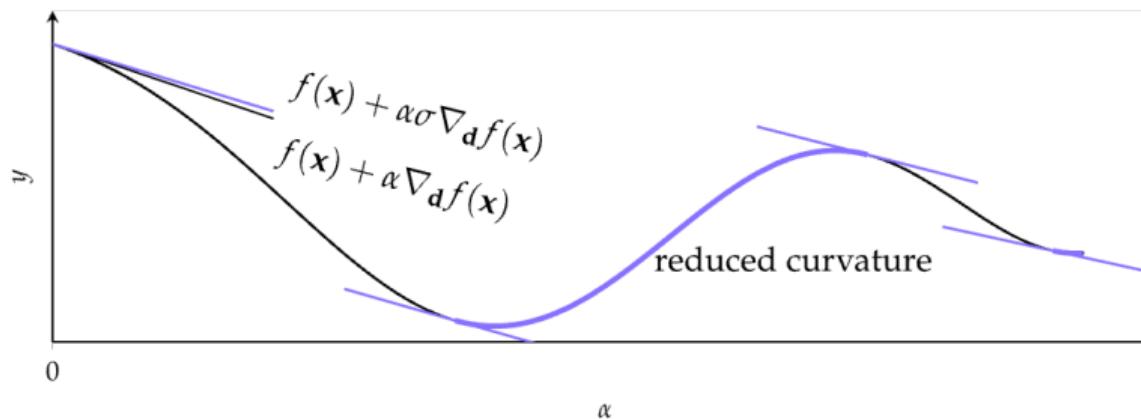
$$\nabla_{\mathbf{d}_k} f(\mathbf{x}_{k+1}) \geq \sigma \nabla_{\mathbf{d}_k} f(\mathbf{x}_k)$$



Approximate Line Search

Regions satisfying the curvature condition $\nabla_{d_k} f(x_{k+1}) \geq \sigma \nabla_{d_k} f(x_k)$

- Consider the univariate function $\phi(\alpha) = f(x_k + \alpha d_k)$.
- 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.



Approximate Line Search: Example

Consider approximate line search on $f(x_1, x_2) = x_1^2 + x_1x_2 + x_2^2$ from $\mathbf{x} = [1, 2]$ in the direction $\mathbf{d} = [-1, -1]$, gradient at \mathbf{x} is $\mathbf{g} = [4, 5]$ 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 ($f(\mathbf{x} + \alpha\mathbf{d}) \leq f(\mathbf{x}) + \beta\alpha(\mathbf{g}^T \cdot \mathbf{d})$):

$$\alpha = 10 : f([1, 2] + 10 \cdot [-1, -1]) \leq 7 + 1 \times 10^{-4} 10 [4, 5]^T [-1, -1] \implies 217 \not\leq 6.991$$

$$\alpha = 10 \cdot 0.5 = 5 : f([1, 2] + 5 \cdot [-1, -1]) \leq 7 + 1 \times 10^{-4} 5 [4, 5]^T [-1, -1] \implies 37 \not\leq 6.996$$

$$\alpha = 2.5 : f([1, 2] + 2.5 \cdot [-1, -1]) \leq 7 + 1 \times 10^{-4} 2.5 [4, 5]^T [-1, -1] \implies 3.25 \leq 6.998$$

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

$$[-3.5, -2.5] \cdot [-1, -1] \geq 0.9 [4, 5] \cdot [-1, -1] \implies 6 \geq -8.1$$

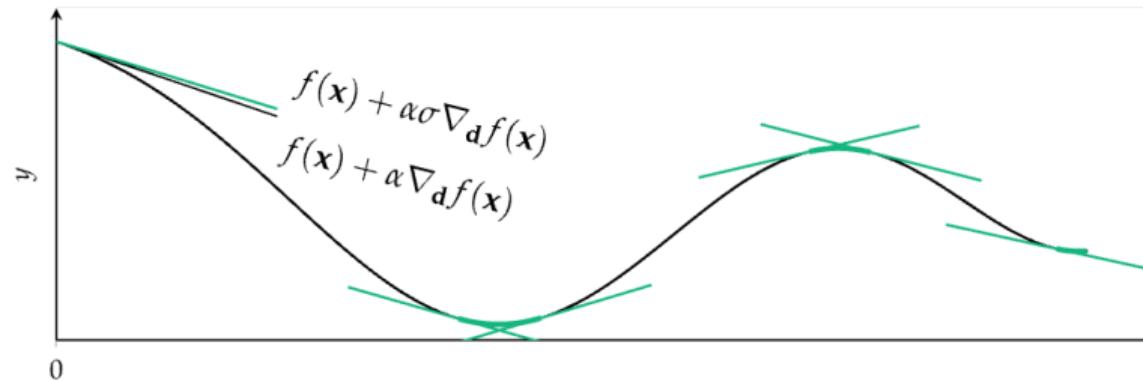
Approximate line search terminates with $\mathbf{x} = [-1.5, -0.5]$.

Approximate Line Search

A step length may satisfy the Wolfe conditions without being particularly close to a minimizer of ϕ . We can modify the curvature condition to force α_k to exclude points that are far from stationary points of ϕ , ie, we no longer allow the derivative $\phi'(\alpha_k)$ to be too positive.

Strong Wolf conditions:

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



Approximate Line Search

- Satisfying the strong Wolfe conditions requires a more complicated algorithm

Strong backtracking line search:

1. Bracketing Phase: tests successively larger step sizes to bracket an interval $[\alpha_{k-1}, \alpha_k]$ guaranteed to contain step lengths satisfying the Wolfe conditions.
2. Zoom Phase: shrink the interval using bisection to find point satisfying the **strong** Wolfe conditions

Approximate Line Search

1. Bracketing Phase

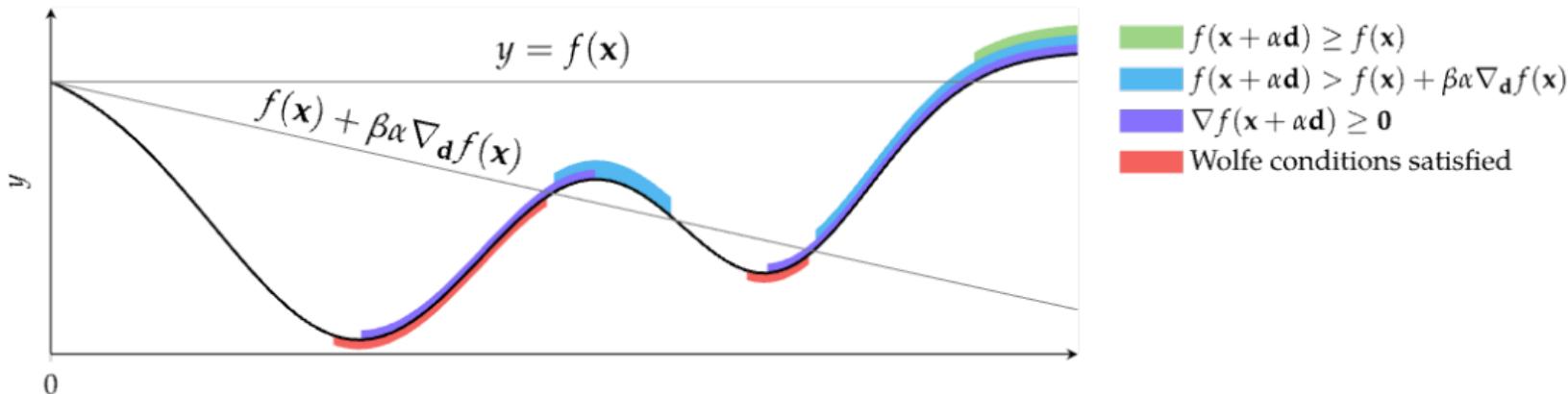
An interval guaranteed to contain step lengths satisfying the Wolfe conditions is found when one of the following conditions hold:

$$f(\mathbf{x} + \alpha \mathbf{d}) \geq f(\mathbf{x})$$

$$f(\mathbf{x} + \alpha \mathbf{d}) > f(\mathbf{x}) + \beta \alpha \nabla_{\mathbf{d}} f(\mathbf{x})$$

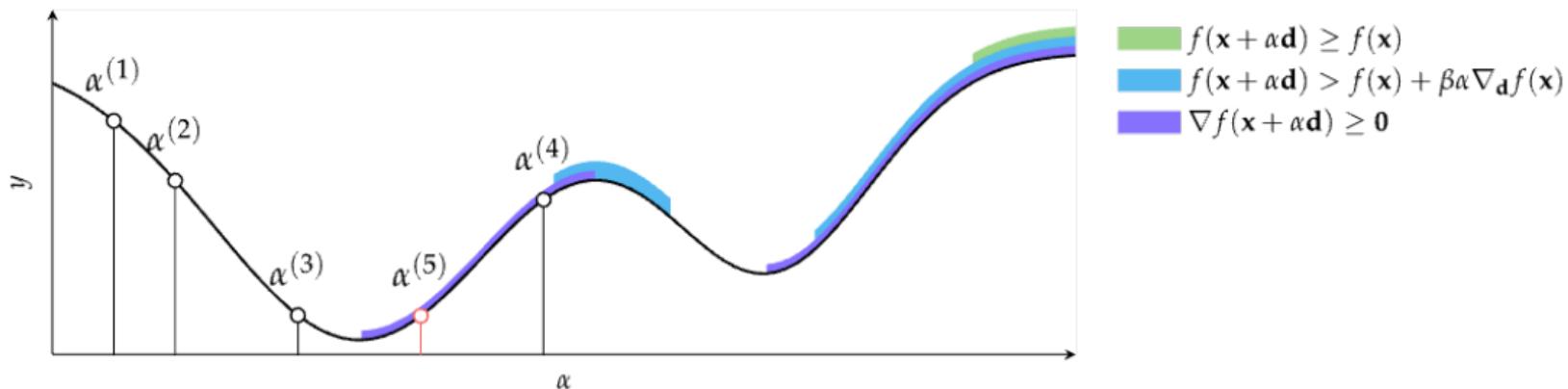
$$\nabla f(\mathbf{x} + \alpha \mathbf{d}) \geq \mathbf{0}$$

Violation of Wolfe conditions



Approximate Line Search

1. Braketing Phase + zoom phase (α_5)



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Convergence Analysis

Convergence of Line Search

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

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

Theorem (Zoutendijk condition)

Consider any iteration of the form $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k + \alpha_k \mathbf{d}_k$, where \mathbf{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 $\mathcal{L} = \{x : f(x) \leq f(\mathbf{x}_0)\}$, where \mathbf{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

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

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.

Rate of Convergence

Let $\{\mathbf{x}_k\}$ be a sequence in \mathbb{R}^n that converges to \mathbf{x}^* .

The convergence is said to be **Q-linear** (quotient-linear) if there is a constant $r \in (0, 1)$ such that

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

ie, the distance to the solution \mathbf{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

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|} = 0$$

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

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

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 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

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

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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

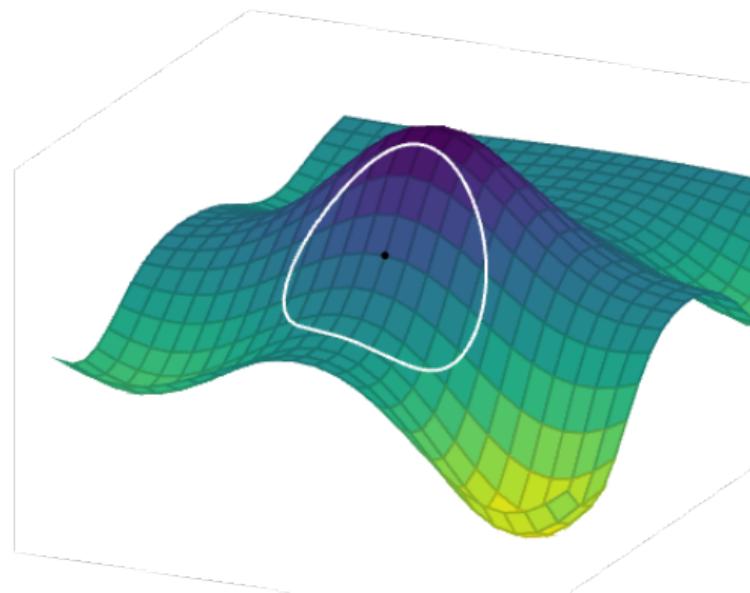
Trust Region Methods

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

$$\text{minimize}_{\mathbf{x}'} \hat{f}(\mathbf{x}')$$

$$\text{subject to } \|\mathbf{x} - \mathbf{x}'\| \leq \delta$$

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



Trust Region Methods

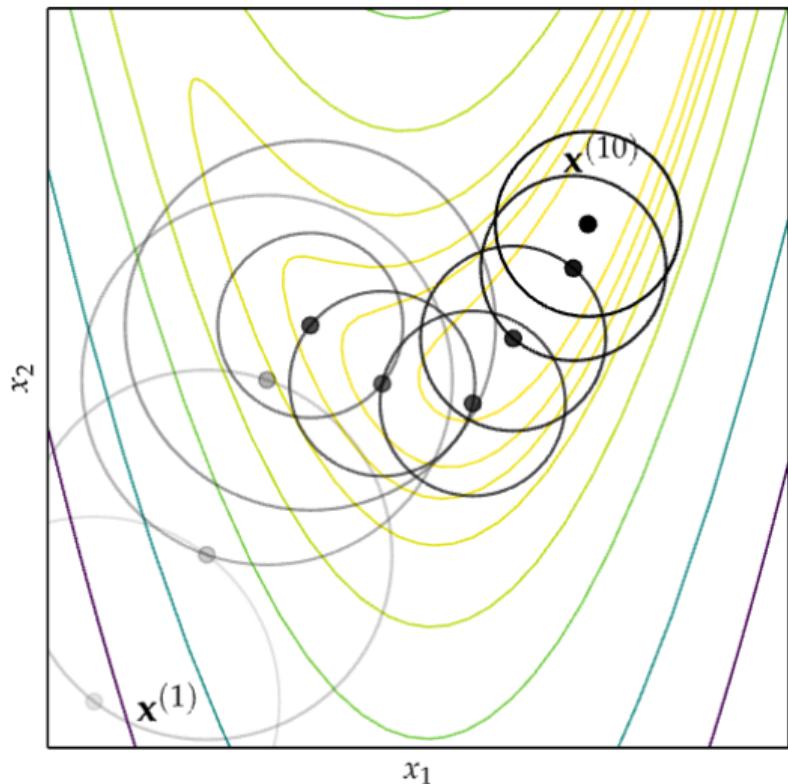
δ can be expanded or contracted based on performance

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

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

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.