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.

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
3. Decide **step size** (= magnitude of the overall step = α_k, since commonly $||\boldsymbol{d}_k||_2 = 1$)
4. Compute next design point $\boldsymbol{x}_{k+1}$

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

Line Search for Step Size

Assuming we have the search direction:

- Used to compute α
- Using the techniques discussed from previous classes, solve:

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

- Often this is computed approximately to reduce cost

Line Search: Alternatives

Step size:

- Fixed α called **learning rate** (commonly $||\boldsymbol{d}_k||_2 = 1$ not imposed)
- **Decaying step factor**

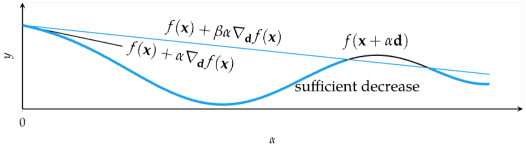
$$\alpha_k = \alpha_1 \gamma^{k-1} \qquad \text{for } \gamma \in [0, 1]$$

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

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

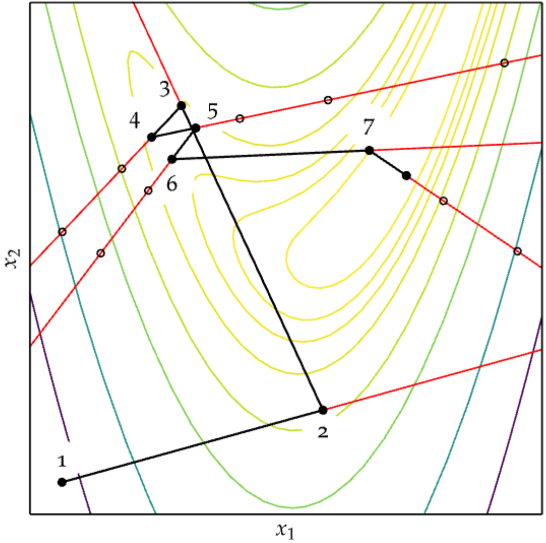


- $\beta \in [0, 1]$, usually $\beta = 1 \times 10^{-4}$

- Backtracking line search starts with a large step and then backs off

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

Approximate Line Search: Example



Approximate Line Search

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

1. First Wolfe Condition: Sufficient Decrease

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

2. Second Wolfe Condition: Curvature Condition

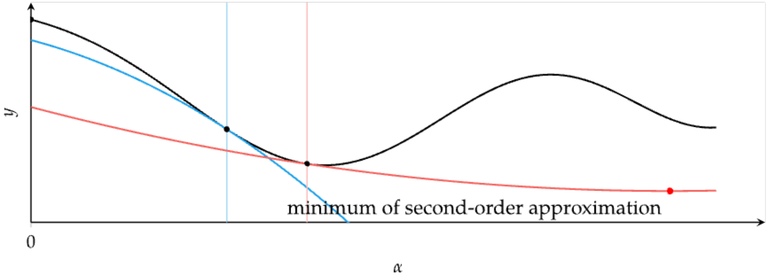
$$\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_{k+1}) \geq \sigma\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)$$

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

Approximate Line Search

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

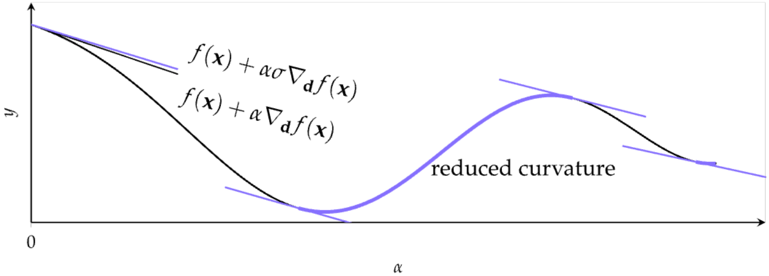
$$\nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_{k+1}) \geq \sigma \nabla_{\boldsymbol{d}_k} f(\boldsymbol{x}_k)$$



Approximate Line Search

Regions satisfying the curvature condition

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



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 $\nabla_{\boldsymbol{d}} f(\boldsymbol{x}') \geq \sigma \nabla_{\boldsymbol{d}} f(\boldsymbol{x})$:

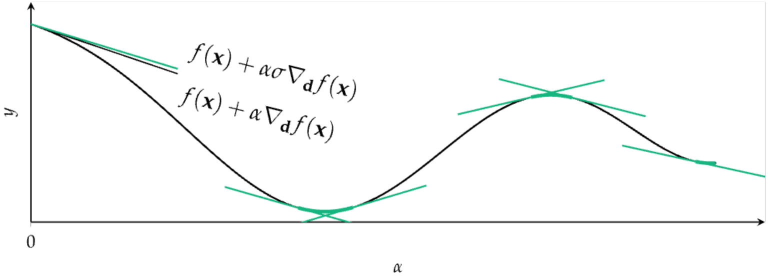
$$[-3.5, -2.5] \cdot [-1, -1] \geq \sigma [4, 5] \cdot [-1, -1] \implies 6 \geq -8.1$$

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

Approximate Line Search

Regions where the strong curvature condition is satisfied

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



Approximate Line Search

- The sufficient decrease condition with the strong curvature condition form the strong Wolfe conditions.

- Satisfying the strong Wolfe conditions requires a more complicated algorithm

  Strong backtracking line search:

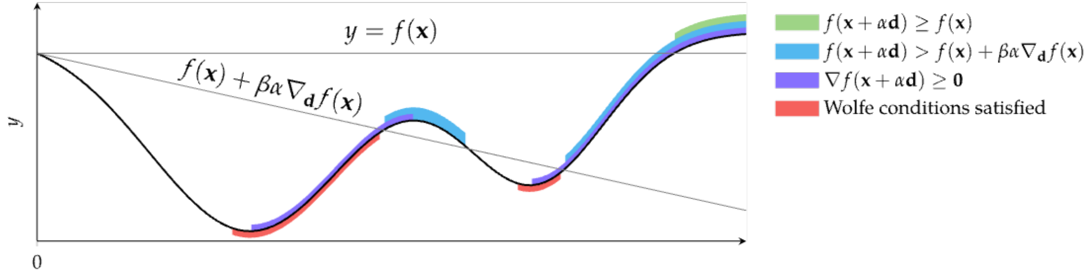
  1. Bracketing Phase: tests successively larger step sizes to bracket an interval $[\alpha_{k-1}, \alpha_k]$ guaranteed to contain step lengths satisfying the Wolfe conditions.
  2. Zoom Phase: shrink the interval using bisection to find point satisfying Wolfe conditions

Approximate Line Search

1. Bracketing Phase

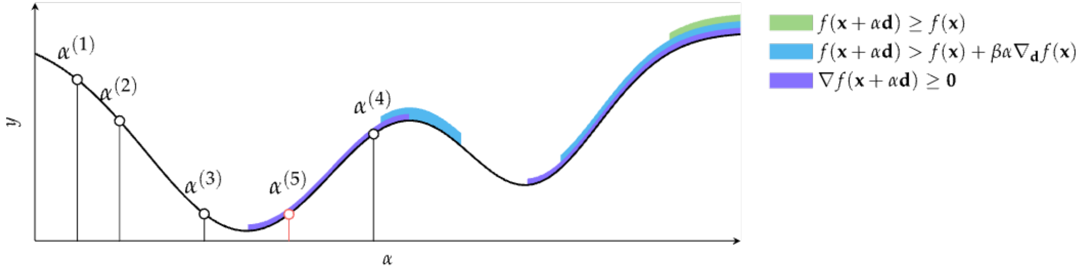
An interval guaranteed to contain step lengths satisfying the Wolfe conditions is found when one of the following conditions hold:

$$f(\boldsymbol{x} + \alpha \boldsymbol{d}) \geq f(\boldsymbol{x})$$
$$f(\boldsymbol{x} + \alpha \boldsymbol{d}) > f(\boldsymbol{x}) + \beta\alpha\nabla \boldsymbol{d} f(\boldsymbol{x})$$
$$\nabla f(\boldsymbol{x} + \alpha \boldsymbol{d}) \geq 0$$



Approximate Line Search

1. Braketing Phase + zoom phase (α_5)



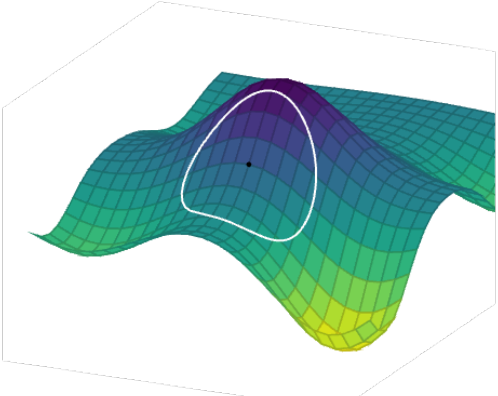
Trust Region Methods

- 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

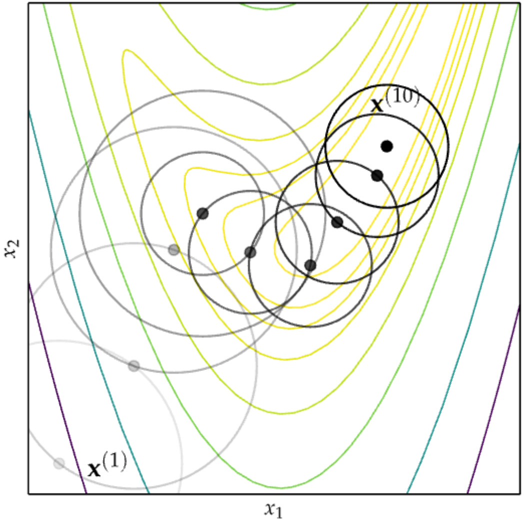
Trust Region Methods

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
if $\eta > \eta_2$ expand

Trust Region Methods: Example



Trust regions can be also non circular.

Trust Region Methods

Termination Conditions (commonly used together):

- Maximum Iterations: $k > k_{\text{max}}$
- 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.