AGEC 652 - Lecture 5.1

Unconstrained optimization

Part B: Line search and trust region methods

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Course roadmap

1. Intro to Scientific Computing
2. Numerical operations and representations
3. Systems of equations
4. Function approximation (Skipped)
5. **Optimization**
    - 5.1 **Unconstrained optimization**
        - A) Theory and derivative-free methods
        - B) **Line-search and trust region methods** $\leftarrow$ *You are here*
    - 5.2 Constrained optimization
6. Structural estimation

*These slides are based on Miranda & Fackler (2002), Nocedal & Wright (2006), Judd (1998), and course materials by Ivan Rudik and Florian Oswald.

Solution strategies: line search vs. trust region

When we move from $x^{(k)}$ to the next iteration, $x^{(k+1)}$, we have to decide

- Which direction from $x^{(k)}$
- How far to go from $x^{(k)}$

There are two fundamental solution strategies that differ in the order of those decisions

- **Line search** methods first choose a *direction* and then select the optimal *step size*
- **Trust region** methods first choose a *step size* and then select the optimal *direction*

Line search algorithms

Line search algorithms

General idea:

1. Start at some current iterate x_k
2. Select a direction to move in p_k
3. Figure out how far along p_k to move

Line search algorithms

How do we figure out how far to move?

"Approximately" solve this problem to figure out the **step length** α

$$\min_{\alpha>0} f(x_k + \alpha p_k)$$

We are finding the distance to move (α) along direction p_k that minimizes our objective f

Typically, algorithms do not perform the full minimization problem since it is costly

- We only try a limited number of step lengths and stop when an approximation criterion is met (ex: Armijo, Wolfe, or Goldstein conditions)

Line search: step length selection

Typical line search algorithms select the step length in two stages

1. Bracketing: pick an interval with desirable step lengths
2. Bisection or interpolation: find a "good" step length in this interval

Line search: step length selection

A widely-used method is the **Backtracking** procedure

1. Choose $\bar{\alpha} > 0, \rho \in (0,1), c \in (0,1)$
2. Set $\alpha \leftarrow \bar{\alpha}$
3. Repeat until $f(x_k + \alpha p_k) \leq f(x_k) + c\alpha \nabla f_k^T p_k$
   - $\alpha \leftarrow \rho\alpha$
4. Terminate with $\alpha_k = \alpha$

- Step 3 checks the *Armijo condition*, which checks for a *sufficient decrease* for convergence

*Several other step lenght methods exist. See Nocedal & Wright Ch.3 and Miranda & Fackler Ch 4.4 for more examples.

Line search: direction choice

We still haven't answered, what direction p_k do we decide to move in?

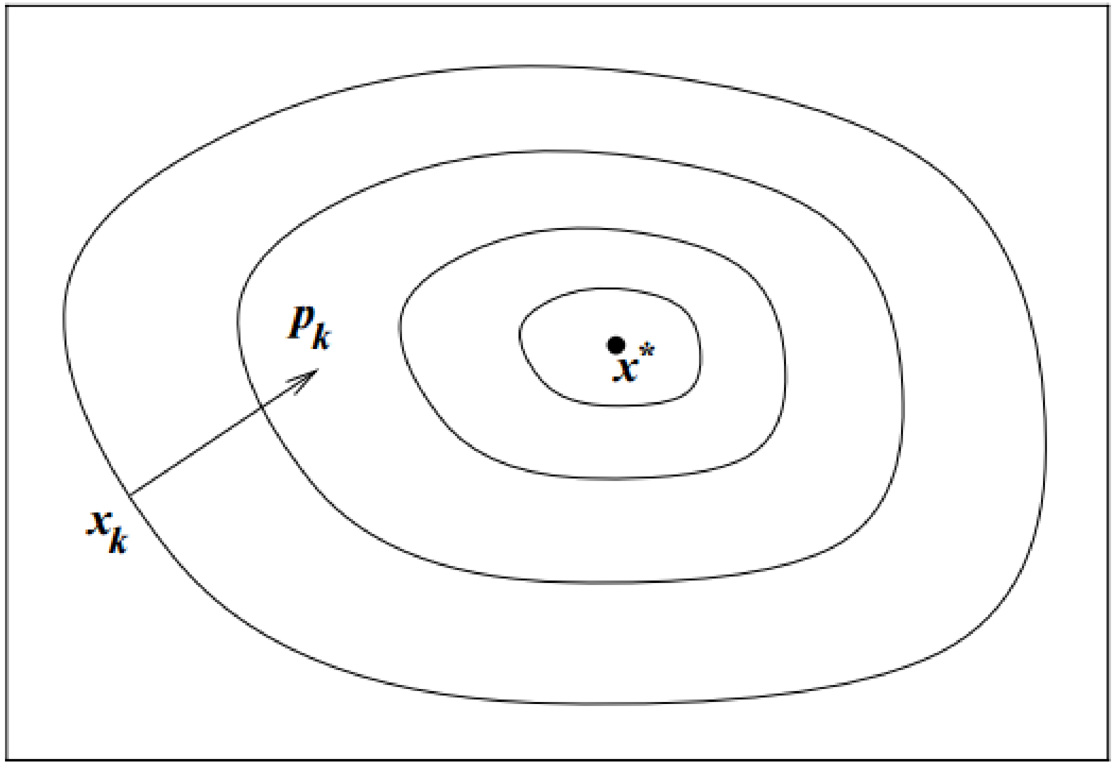
What's an obvious choice for p_k?

The direction that yields the *steepest descent*

$-\nabla f_k$ is the direction that makes f decrease most rapidly

- k indicates we are evaluating f at iteration k

Steepest descent method



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Steepest descent method

We can verify this is the direction of steepest descent by referring to Taylor's theorem

For any direction p and step length α, we have that

$$f(x_k + \alpha p) = f(x_k) + \alpha\, p^T \nabla f_k + \frac{1}{2!}\, \alpha^2 p^T \nabla^2 f(x_k + tp)\, p$$

The rate of change in f along p at x_k $(\alpha = 0)$ is $p^T \nabla f_k$

Steepest descent method

The the unit vector of quickest descent solves

$$\min_{p} p^T \nabla f_k \quad \text{subject to: } ||p|| = 1$$

Re-express the objective as

$$\min_{\theta, ||p||} ||p|| \, ||\nabla f_k|| cos \, \theta$$

where θ is the angle between p and ∇f_k

The minimum is attained when $cos \, \theta = -1$ and $p = -\frac{\nabla f_k}{||\nabla f_k||}$, so the direction of steepest descent is simply $-\nabla f_k$

Steepest descent method

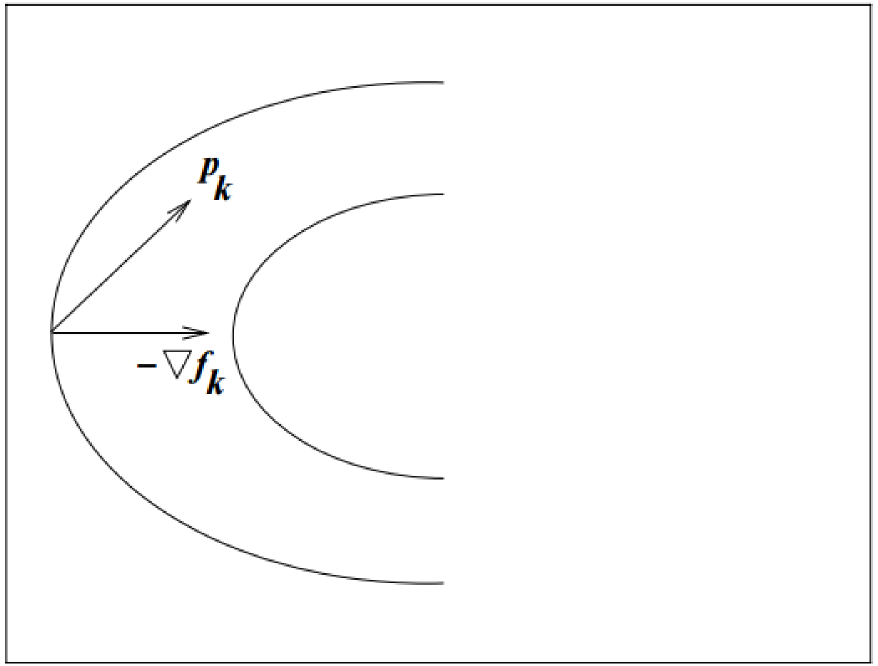
The **steepest descent method** searches along this direction at every iteration k

- It may select the step length α_k in several different ways
- A benefit of the algorithm is that we only require the gradient of the function, and no Hessian
- However it can be very slow

Line search: alternative directions

We can always use search directions other than the steepest descent

Any descent direction (i.e. one with angle strictly less than 90° of $-\nabla f_k$) is *guaranteed* to produce a decrease in f as long as the step size is sufficiently small



But is $-\nabla f_k$ always the best search direction?

Newton-Raphson method

The most important search direction is not steepest descent but **Newton's direction**

This direction gives rise to the Newton-Raphson Method

- This method is basically just using Newton's method to find the root of the gradient of the objective function

Newton-Raphson method

Newton's direction comes out of the second order Taylor series approximation to $f(x_k + p)$

$$f(x_k + p) \approx f_k + p^T \nabla f_k + \frac{1}{2!} p^T \nabla^2 f_k p$$

We find the Newton direction by selecting the vector p that minimizes $f(x_k + p)$

This ends up being

$$p_k^N = -[\nabla^2 f_k]^{-1} \nabla f_k$$

Newton-Raphson method

The algorithm is pretty much the same as in Newton's rootfinding method

1. Start with an initial guess x_0
2. Repeat until convergence
   - $x_{k+1} \leftarrow x_k - \alpha_k [\nabla^2 f_k]^{-1} \nabla f_k$
     - where α_k comes from a step length selection algorithm
3. Terminate with $x^* = x_k$

- Most packages just use $\alpha = 1$ (i.e., Newton's method step). But you can usually change this parameter if you have convergence issues

Newton-Raphson method

This approximation to the function we are trying to solve has error of $O(||p||^3)$, so if p is small, the quadratic approximation is very accurate

Drawbacks:

- The Newton direction is only guaranteed to decrease the objective function if $\nabla^2 f_k$ is positive definite
- It requires explicit computation of the Hessian, $\nabla^2 f(x)$
  - But quasi-Newton solvers also exist

Quasi-Newton methods

Just like in rootfinding, there are several methods to avoid computing derivatives (Hessians, in this case)

Instead of the true Hessian $\nabla^2 f(x)$, these methods use an approximation B_k (to the inverse of the Hessian). Hence, they set direction

$$d_k = -B_k \nabla f_k$$

The optimization method analogous to Broyden's that also uses the *secant condition* is the **BFGS method**

- Named after its inventors, Broyden, Fletcher, Goldfarb, Shanno

Linear search methods in Julia

Once again, we will use `Optim.jl`. We'll see an example with an easy function, solving it using Steepest Descent, Newton-Raphson, and BFGS

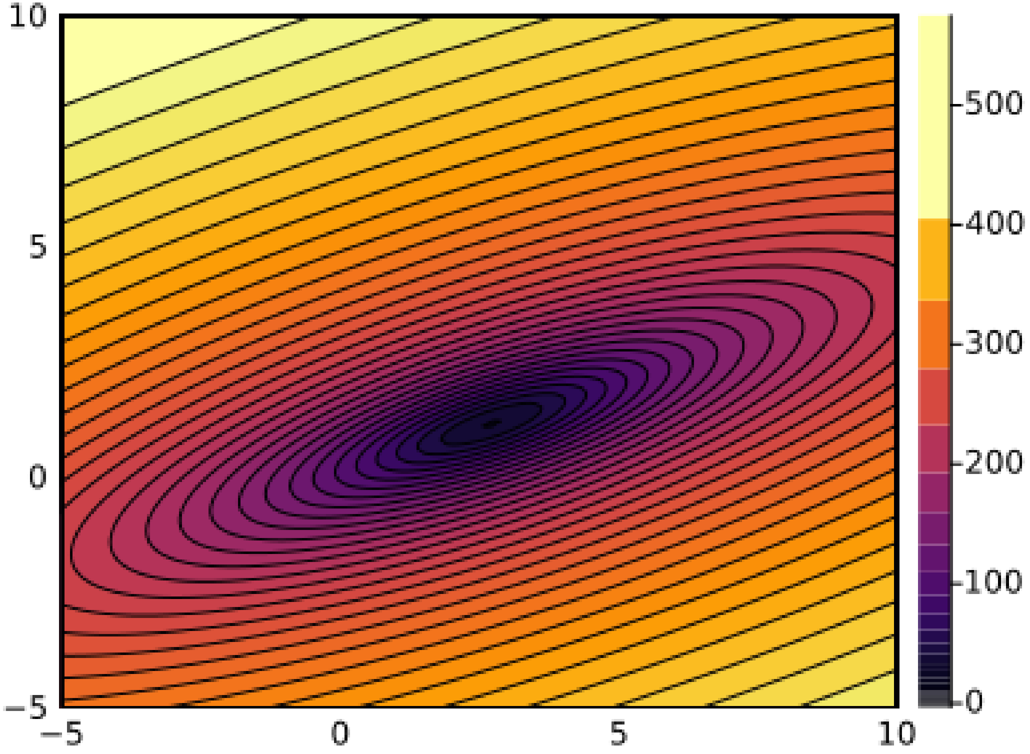
$$f(x_1, x_2) = ax_1^2 + bx_2^2 + cx_1 + dx_2 + ex_1x_2$$

We will use parameters $a = 1, b = 4, c = -2, d = -1, e = -3$

```julia
using Optim, Plots, LinearAlgebra;
a = 1; b = 4; c = -2; d = -1; e = -3;
f(x) = a*x[1]^2 + b*x[2]^2 + c*x[1] + d*x[2] + e*x[1]*x[2];
```

Linear search methods in Julia

Let's take a look at our function with a contour plot



Linear search methods in Julia

Since we will use Newton-Raphson, we should define the gradient and the Hessian of our function

```
# Gradient
function g!(G, x)
    G[1] = 2a*x[1] + c + e*x[2]
    G[2] = 2b*x[2] + d + e*x[1]
end;

# Hessian
function h!(H, x)
    H[1,1] = 2a
    H[1,2] = e
    H[2,1] = e
    H[2,2] = 2b
end;
```

Linear search methods in Julia

Let's check if the Hessian satisfies it being positive semidefinite. One way is to check whether all eigenvalues are positive. In this case, H is constant, so it's easy to check

```
H = zeros(2,2);
h!(H, [0 0]);
LinearAlgebra.eigen(H).values
```

```
## 2-element Vector{Float64}:
##  0.7573593128807148
##  9.242640687119286
```

Linear search methods in Julia

Since the gradient is linear, it is also easy to calculate the minimizer analytically. The FOC is just a linear equation

```
analytic_x_star = [2a e; e 2b]\[-c ;-d]
```

```
## 2-element Vector{Float64}:
##  2.714285714285715
##  1.142857142857143
```

Linear search methods in Julia

Let's solve it with the Steepest (or Gradient) descent method

```
# Initial guess
x0 = [0.2, 1.6];
res_GD = Optim.optimize(f, g!, x0, GradientDescent(), Optim.Options(x_abstol=1e-3))
```

```
##  * Status: success
##
##  * Candidate solution
##     Final objective value:     -3.285714e+00
##
##  * Found with
##     Algorithm:     Gradient Descent
##
##  * Convergence measures
##     |x - x'|               = 4.55e-04 ≤ 1.0e-03
##     |x - x'|/|x'|          = 1.68e-04 ≰ 0.0e+00
##     |f(x) - f(x')|         = 1.25e-06 ≰ 0.0e+00
##     |f(x) - f(x')|/|f(x')| = 3.80e-07 ≰ 0.0e+00
##     |g(x)|                 = 4.83e-04 ≰ 1.0e-08
##
##  * Work counters
```

Linear search methods in Julia

Let's solve it with the Steepest (or Gradient) descent method

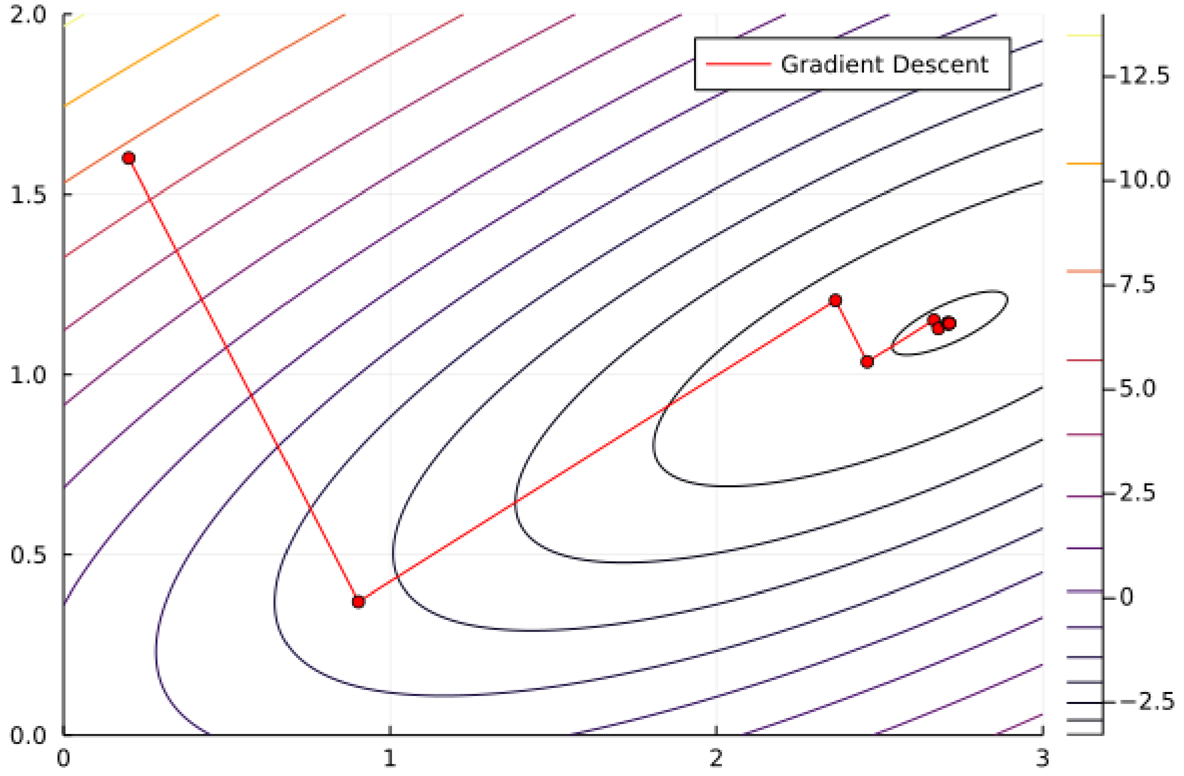
```
res_GD.minimizer
```

```
## 2-element Vector{Float64}:
##  2.7136160576693604
##  1.1425715540060508
```

```
res_GD.minimum
```

```
## -3.285714084769726
```

Linear search methods in Julia



Linear search methods in Julia

We haven't really specified a line search method yet

In most cases, `Optim.jl` will use by default the *Hager-Zhang method*

- This is based on Wolfe conditions

But we can specify other approaches. We need the `LineSearches` package to do that:

```
using LineSearches;
```

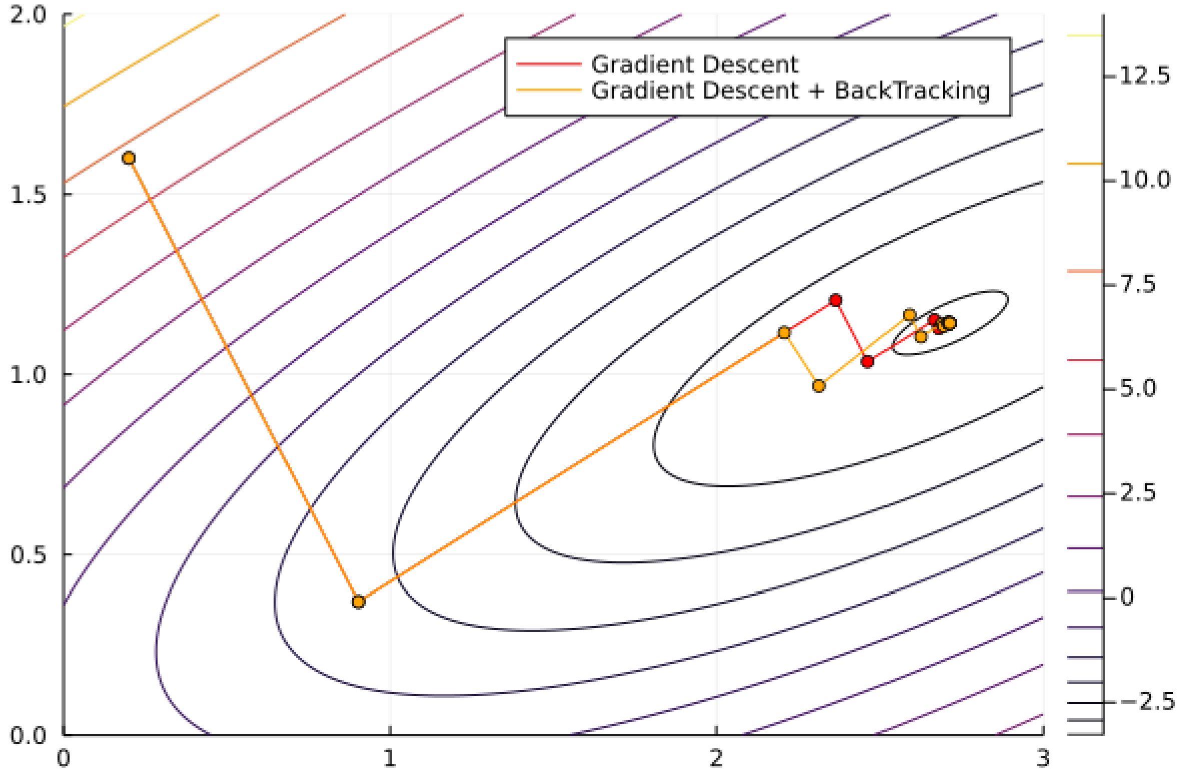
Let's re-run the `GradientDescent` method using $\bar{\alpha} = 1$ and the backtracking method

Linear search methods in Julia

```
Optim.optimize(f, g!, x0,
               GradientDescent(alphaguess = LineSearches.InitialStatic(alpha=1.0),
                               linesearch = BackTracking()),
               Optim.Options(x_abstol=1e-3))
```

```
##  * Status: success
##
##  * Candidate solution
##     Final objective value:     -3.285714e+00
##
##  * Found with
##     Algorithm:     Gradient Descent
##
##  * Convergence measures
##     |x - x'|               = 3.61e-04 ≤ 1.0e-03
##     |x - x'|/|x'|          = 1.33e-04 ≰ 0.0e+00
##     |f(x) - f(x')|         = 8.65e-07 ≰ 0.0e+00
##     |f(x) - f(x')|/|f(x')| = 2.63e-07 ≰ 0.0e+00
##     |g(x)|                 = 6.73e-04 ≰ 1.0e-08
##
##  * Work counters
##     Seconds run:   0  (vs limit Inf)
##     Iterations:    11
```

Linear search methods in Julia



Linear search methods in Julia

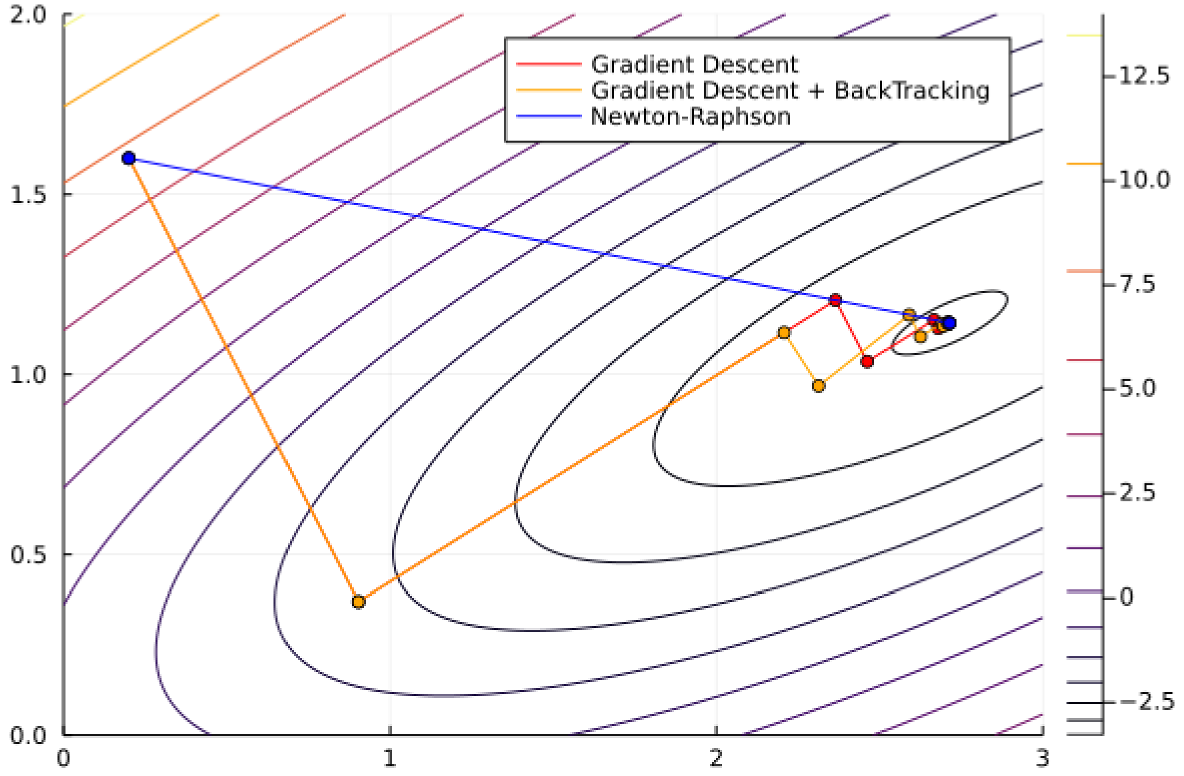
Next, let's use the Newton-Raphson method with default (omitted) line search parameters

- If you omit `g!` and `h!`, `Optim` will approximate them numerically for you. You can also specify options to use auto differentiation

```
Optim.optimize(f, g!, h!, x0, Newton())
```

```
##  * Status: success
##
##  * Candidate solution
##     Final objective value:     -3.285714e+00
##
##  * Found with
##     Algorithm:     Newton's Method
##
##  * Convergence measures
##     |x - x'|               = 2.51e+00 ≰ 0.0e+00
##     |x - x'|/|x'|          = 9.26e-01 ≰ 0.0e+00
##     |f(x) - f(x')|         = 1.06e+01 ≰ 0.0e+00
```

Linear search methods in Julia



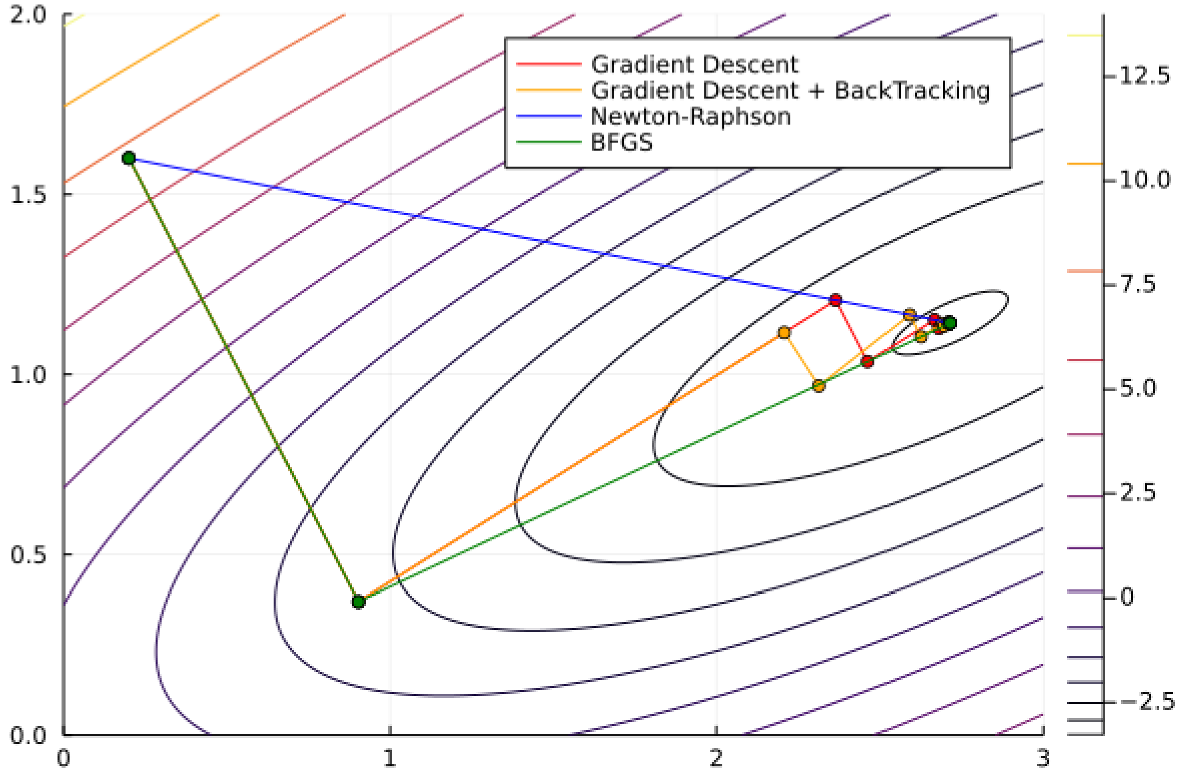
Linear search methods in Julia

Lastly, let's use the BFGS method

```
Optim.optimize(f, x0, BFGS())
```

```
##  * Status: success
##
##  * Candidate solution
##     Final objective value:     -3.285714e+00
##
##  * Found with
##     Algorithm:     BFGS
##
##  * Convergence measures
##     |x - x'|               = 1.81e+00 ≰ 0.0e+00
##     |x - x'|/|x'|          = 6.67e-01 ≰ 0.0e+00
##     |f(x) - f(x')|         = 1.47e+00 ≰ 0.0e+00
##     |f(x) - f(x')|/|f(x')| = 4.48e-01 ≰ 0.0e+00
##     |g(x)|                 = 1.28e-10 ≤ 1.0e-08
##
##  * Work counters
##     Seconds run:   0  (vs limit Inf)
##     Iterations:    2
```

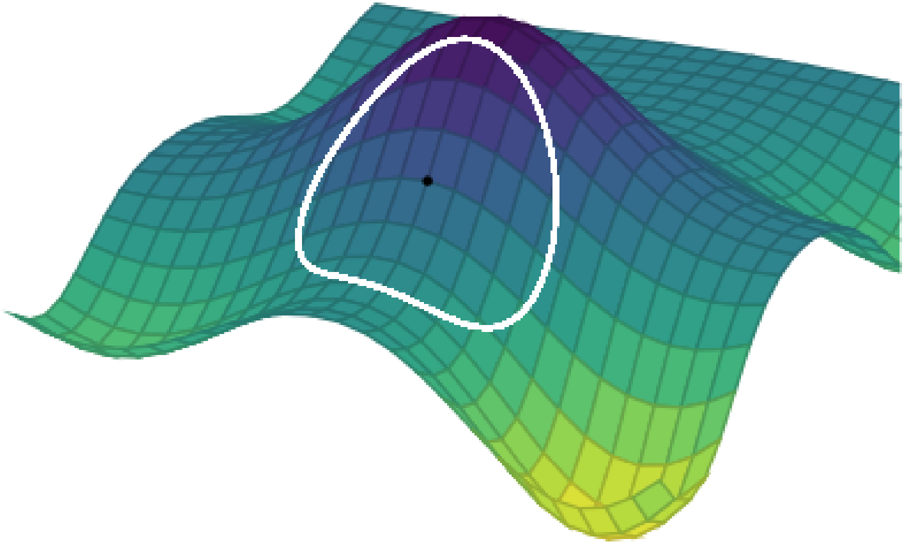
Linear search methods in Julia



Trust regions algorithms

Trust region methods

Trust region methods construct an approximating model, m_k whose behavior near the current iterate x_k is close to that of the actual function f



We then search for a minimizer of m_k

Trust region methods

Issue: m_k may not represent f well when far away from the current iterate x_k

Solution: Restrict the search for a minimizer to be within some region of x_k, called a **trust region**

We are only going to cover the basic of trust region methods. For details, see Nocedal & Wright (2006), Chapter 4.

Trust region methods

Trust region problems can be formulated as

$$\min_{p} m_k(x_k + p)$$

where $x_k + p \in \Gamma$

- Γ is a ball defined by $||p||_2 \leq \Delta_k$
- Δ_k is called the trust region radius

Δ_k is adjusted every iteration based on how well m_k approximates f_k around current guess x_k

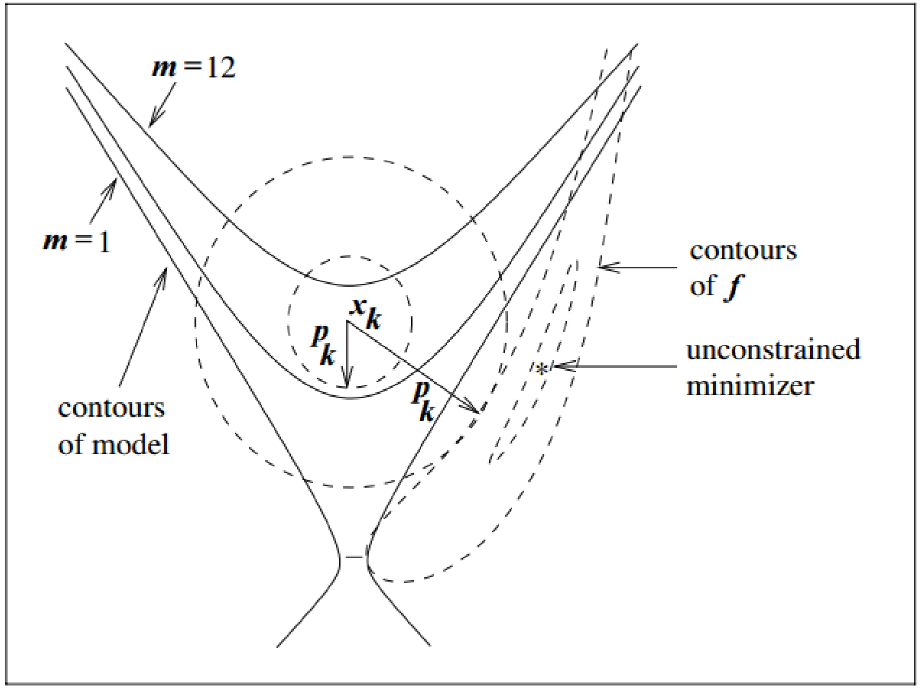
Trust region methods

Typically the approximating model m_k is a quadratic function (i.e. a second-order Taylor approximation)

$$m_k(x_k + p) = f_k + p^T \nabla f_k + \frac{1}{2!} p^T B_k p$$

where B_k is the Hessian or an approximation to the Hessian

Solving this problem usually involves finding the *Cauchy point*



Trust region methods

From x_k, the Cauchy point can be found in the direction

$$p_k^C = -\tau_k \frac{\Delta_k}{||\nabla f_k||} \nabla f_k$$

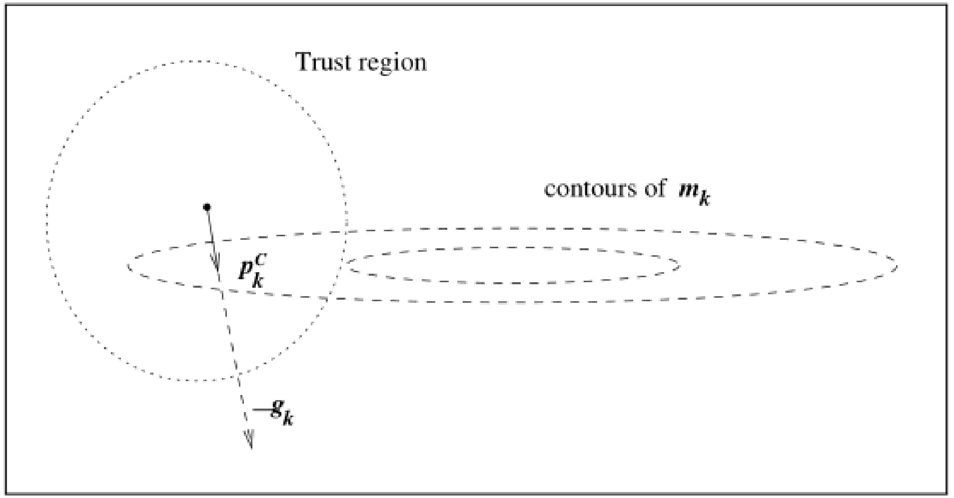


Figure 4.3 The Cauchy point.

So it's kind of a gradient descent ($-\nabla f_k$), but with an adjusted step size within the trust region. The step size depends on the radius Δ_k and parameter τ_k

$$\tau_k = \begin{cases} 1 & \text{if } \nabla f_k^T B_k \nabla f_k \leq 0 \\ \min(||\nabla f_k||^3 / \Delta_k \nabla f_k^T B_k \nabla f_k, 1) & \text{otherwise} \end{cases}$$

Trust region methods

If you ran `nlsolve` with default parameters, you may have noticed it uses `Trust region with dogleg`. What's the deal with the `dogleg`?

It's an improvement on the Cauchy point method

- It allows us to move in V-shaped trajectory instead of slowly adjusting with Cauchy directions along a curved path

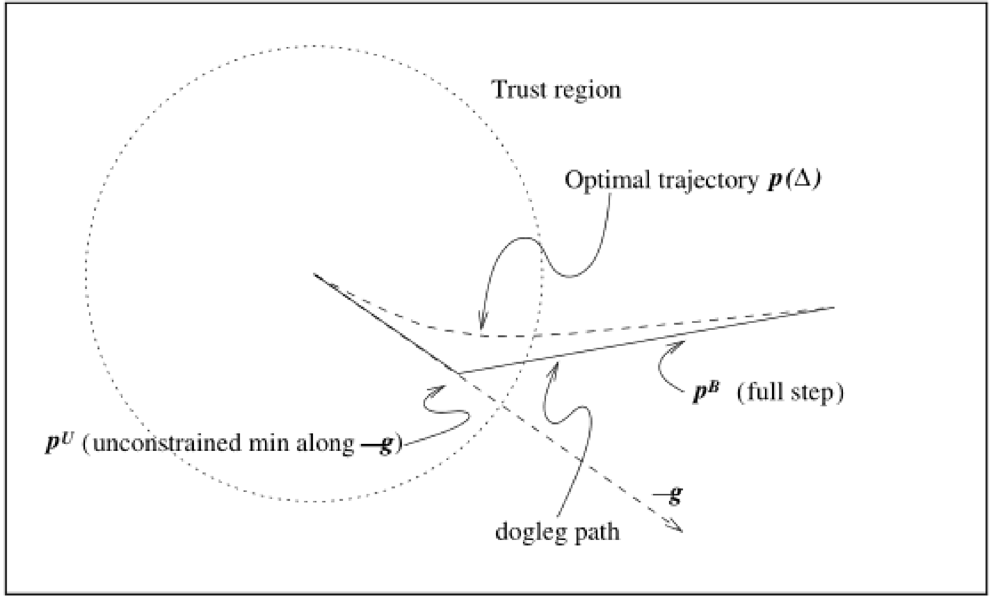


Figure 4.4 Exact trajectory and dogleg approximation.

Trust region method illustration

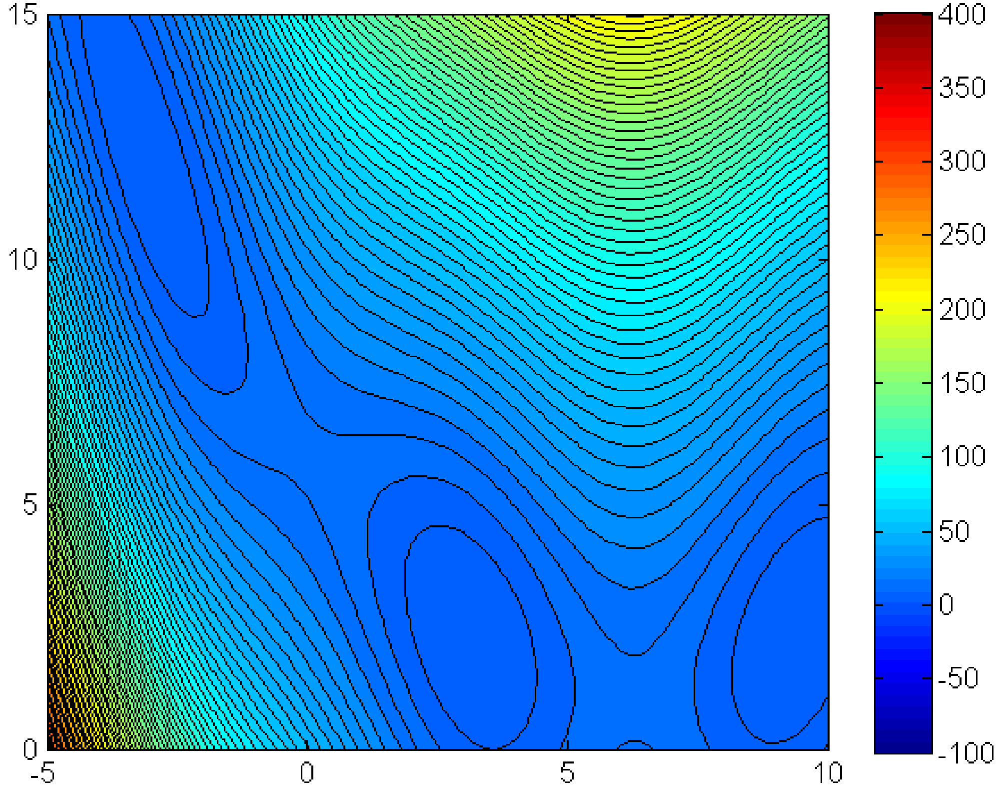
Let's see an illustration of the trust region method with the Branin function (it has 3 global minimizers)*

$$min f(x_1, x_2) = (x_2 - 0.129x_1^2 + 1.6x_1 - 6)^2 + 6.07\cos(x_1) + 10$$

- Source for this example: https://optimization.mccormick.northwestern.edu/index.php/Trust-region_methods

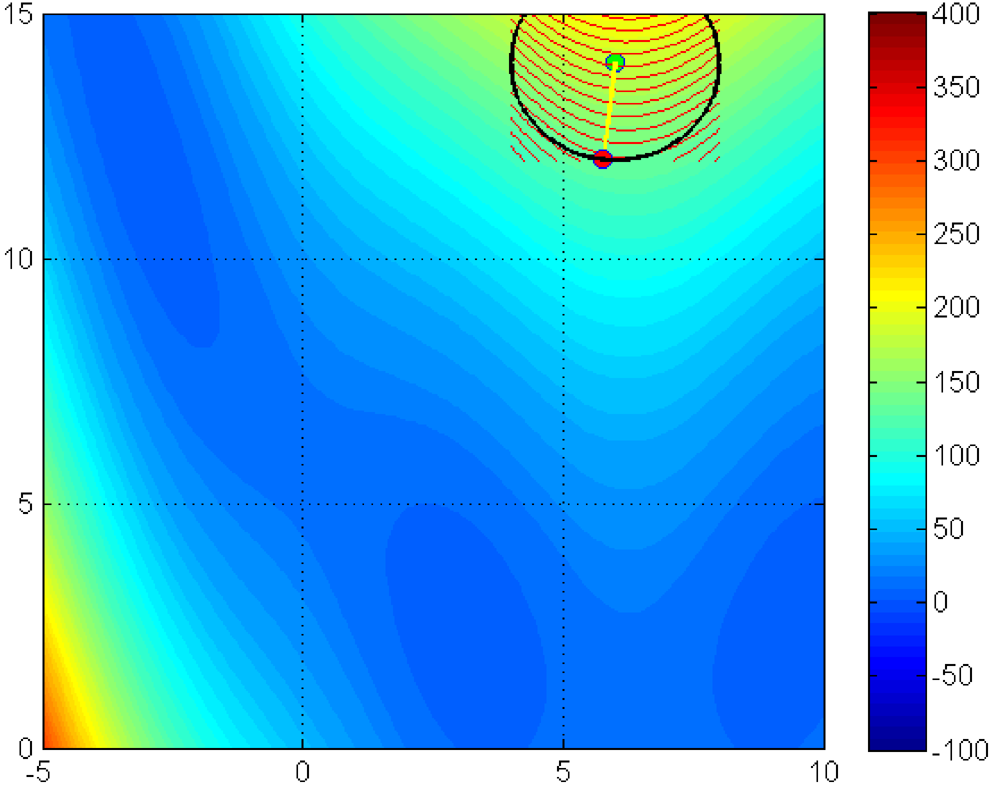
Trust region method illustration

Contour plot



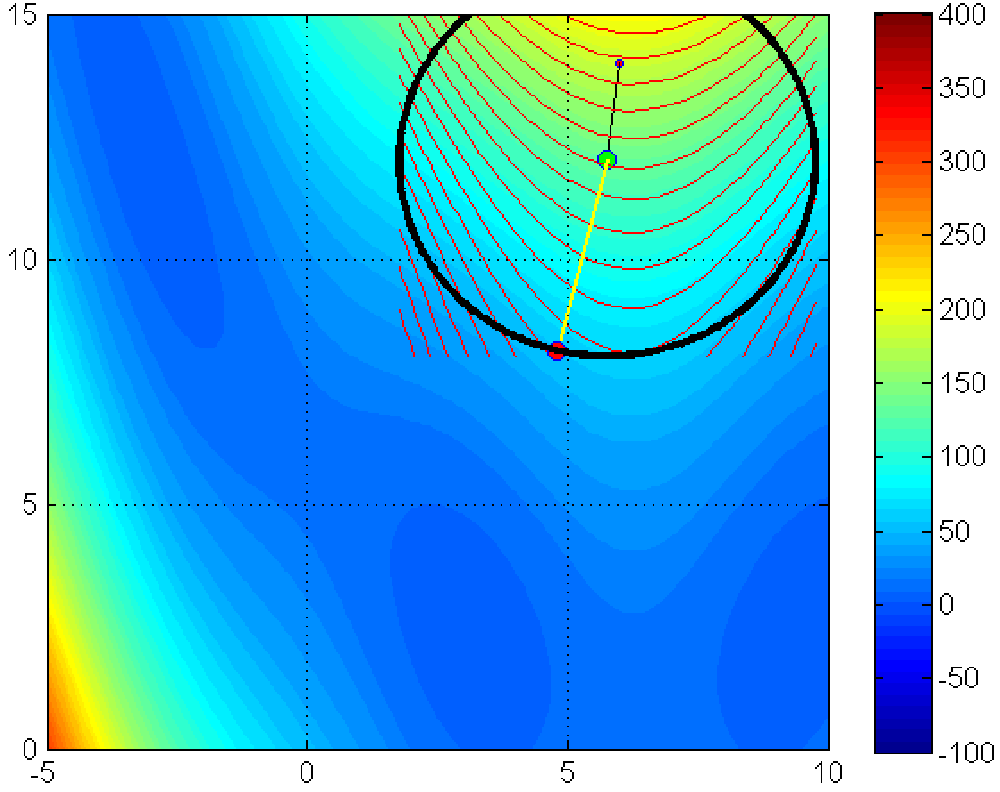
Trust region method illustration

Iteration 1



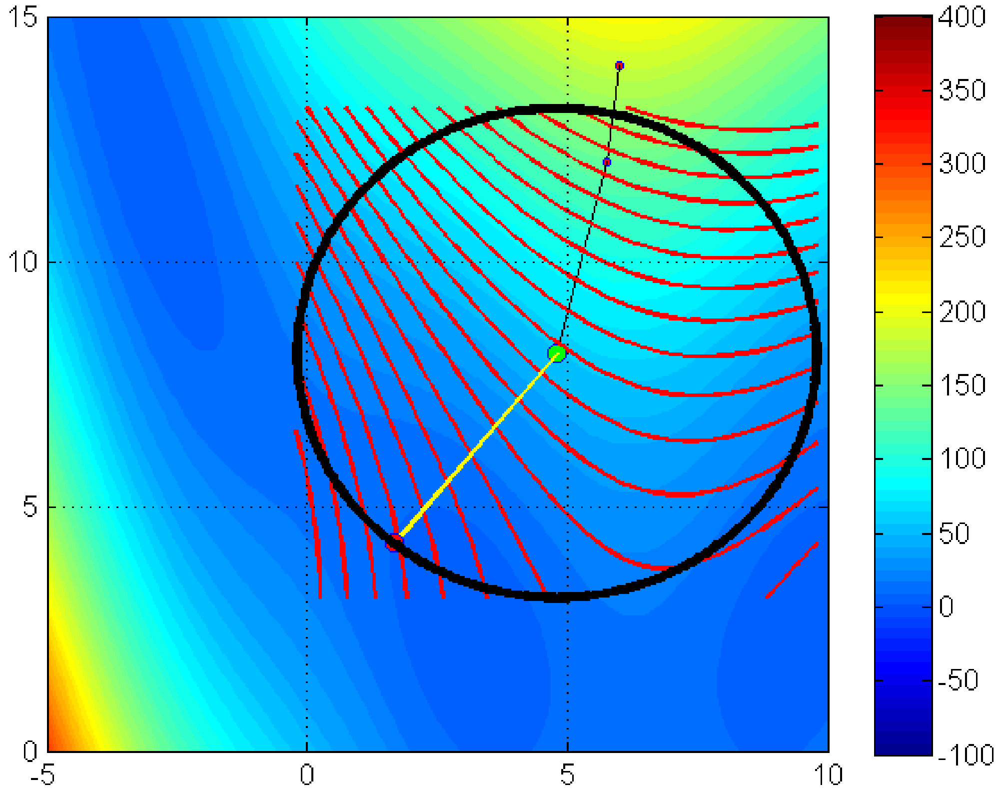
Trust region method illustration

Iteration 2



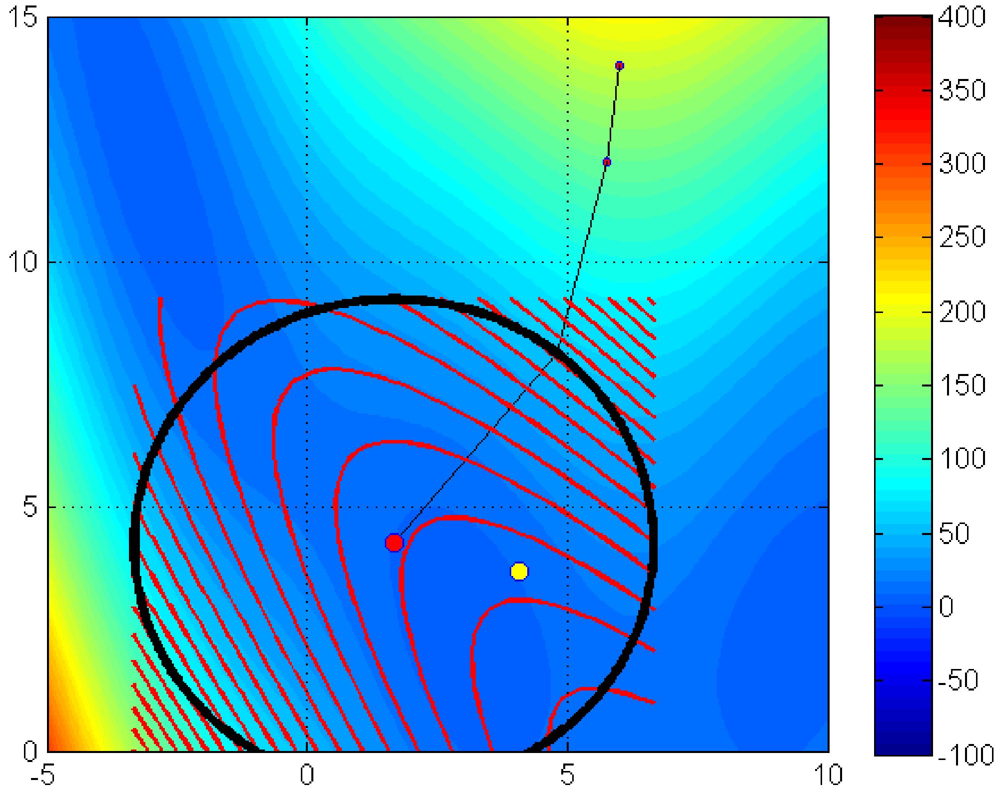
Trust region method illustration

Iteration 3



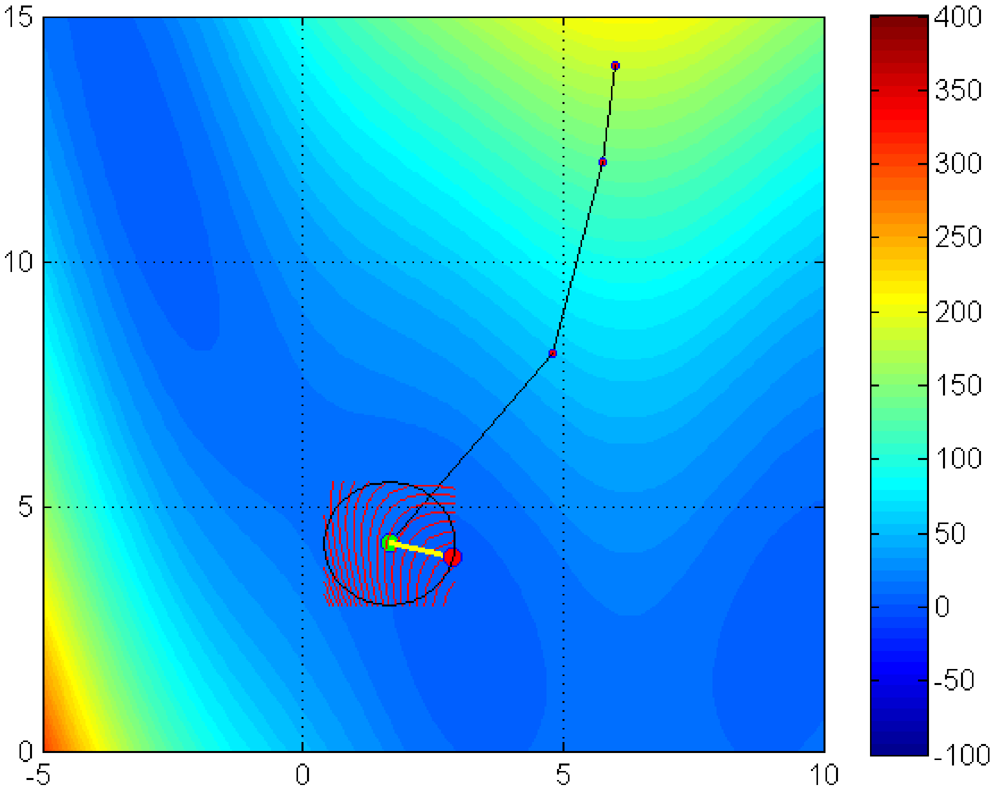
Trust region method illustration

Iteration 4



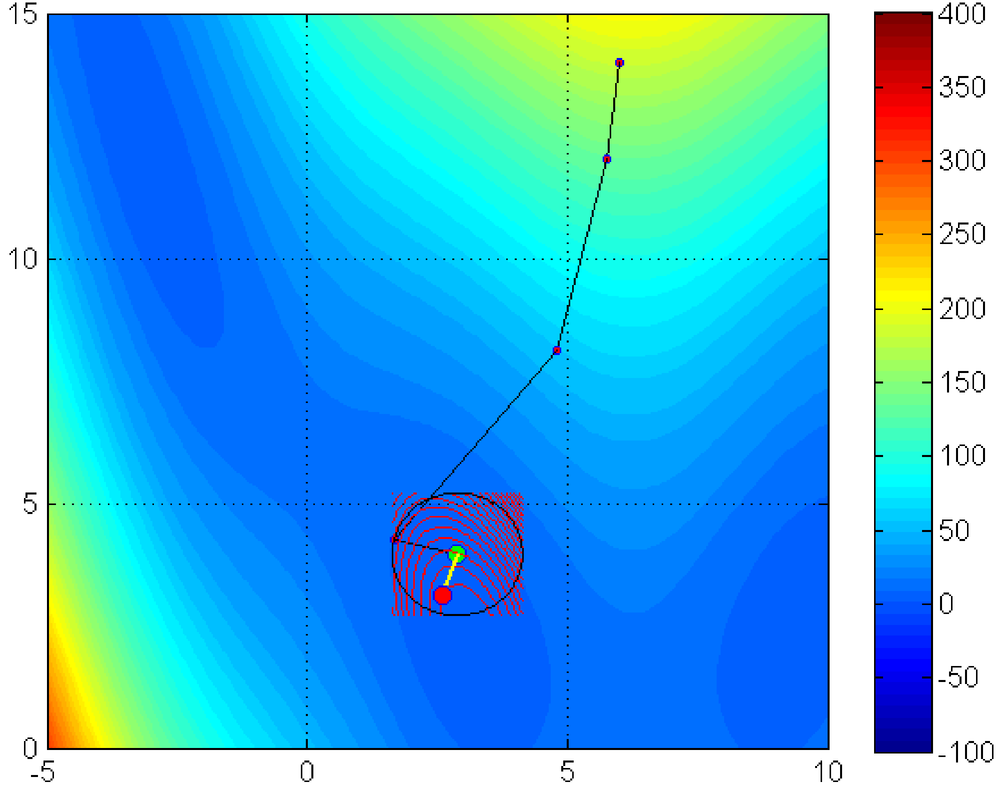
Trust region method illustration

Iteration 5



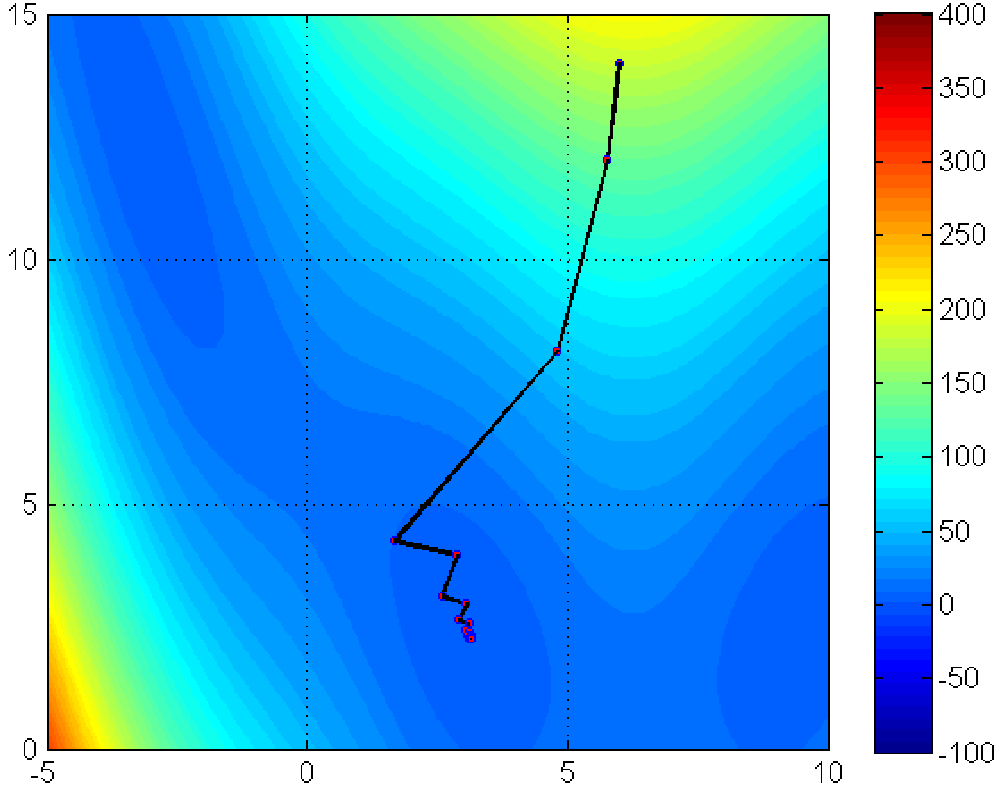
Trust region method illustration

Iteration 6



Trust region method illustration

Full trajectory



Trust region methods in Julia

`Optim` includes a `NewtonTrustRegion()` solution method. To use it, you can call `optimize` just like you did with `Newton()`

Your turn: Trust region methods in Julia

Use `Optim` and `NewtonTrustRegion`* to solve the same quadratic function from before

$$f(x_1, x_2) = ax_1^2 + bx_2^2 + cx_1 + dx_2 + ex_1x_2$$

With parameters $a = 1, b = 4, c = -2, d = -1, e = -3$

```
a = 1; b = 4; c = -2; d = -1; e = -3;
f(x) = a*x[1]^2 + b*x[2]^2 + c*x[1] + d*x[2] + e*x[1]*x[2];
# Complete the arguments of the call
Optim.optimize(<?>, <?>, <?>, <?>, <?>)
```

*Use default parameters. You can tweak solver parameters later by checking out the documentation
https://julianlsolvers.github.io/Optim.jl/stable/#algo/newton_trust_region/

Trust region methods in Julia

```
##  * Status: success
##
##  * Candidate solution
##     Final objective value:     -3.285714e+00
##
##  * Found with
##     Algorithm:     Newton's Method (Trust Region)
##
##  * Convergence measures
##     |x - x'|               = 1.85e+00 ≰ 0.0e+00
##     |x - x'|/|x'|          = 6.83e-01 ≰ 0.0e+00
##     |f(x) - f(x')|         = 2.15e+00 ≰ 0.0e+00
##     |f(x) - f(x')|/|f(x')| = 6.54e-01 ≰ 0.0e+00
##     |g(x)|                 = 8.88e-16 ≤ 1.0e-08
##
##  * Work counters
##     Seconds run:   0  (vs limit Inf)
##     Iterations:    2
##     f(x) calls:    3
##     ∇f(x) calls:   3
##     ∇²f(x) calls:  3
```

Trust region methods in Julia