

# Lecture 4

## Optimization

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# Software and stuff

Necessary things to do:

- Install the QuantEcon Julia package
- Install the Optim or NLOpt Julia packages

# Optimization

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Some are harder than others:

- Individual utility max: easy
- Decentralized electricity market with nodal pricing and market power: hard
- One input profit maximization problem: easy
- N-input profit maximization with learning and forecasts: hard

# Things we will do

1. Linear rootfinding
2. Non-linear rootfinding
3. Complementarity problems
4. Non-linear unconstrained maximization/minimization
5. Non-linear constrained maximization/minimization

# Linear rootfinding

How do we solve these?

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Consider a simple generic problem:

$$Ax = b$$

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$$x = A^{-1}b$$

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Fixed point problems are rootfinding problems:

$$g(x) = x \Rightarrow f(x) \equiv g(x) - x = 0$$

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$$x_i > a_i \Rightarrow f_i(x) \geq 0 \quad \forall i = 1, \dots, n$$

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What do these equations mean?

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If the constraints on  $x_i$  do not bind,  $a_i < x_i < b_i$ , then the first-order condition is precisely zero

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If the constraints on  $x_i$  do not bind,  $a_i < x_i < b_i$ , then the first-order condition is precisely zero

Suppose the upper bound binds,  $x_i = b_i$

Then  $f_i(x) \geq 0$  since  $x_i > a_i$ , but we can't guarantee that  $f_i(x) = 0$  because  $f_i(x)$  might still be increasing

# Basic non-linear rootfinders: Bisection method

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Continually bisect the interval!

**Write out the code to do it**

# The bisection algorithm

```
function bisection(f, lower_bound, upper_bound)
    tolerance = 1e-3                                # tolerance for solution
    guess = 0.5*(upper_bound + lower_bound)          # initial guess, bisect the interval
    difference = (upper_bound - lower_bound)/2        # initialize bound difference

    while difference > tolerance                   # loop until convergence
        println("Intermediate guess of $guess.")
        difference = difference/2
        if sign(f(lower_bound)) = sign(f(guess))      # if the guess has the same sign as the lower bound
            lower_bound = guess                         # solution is in the upper half of the interval
            guess = guess + difference
        else                                         # else the solution is in the lower half of the interval
            upper_bound = guess
            guess = guess - difference
        end
    end
    println("The root of f(x) is at $guess.")
end;
```

# The bisection method

```
f(x) = x^3
```

```
## f (generic function with 1 method)
```

```
bisection(f, -4, 1)
```

```
## Intermediate guess of -1.5.  
## Intermediate guess of -0.25.  
## Intermediate guess of 0.375.  
## Intermediate guess of 0.0625.  
## Intermediate guess of -0.09375.  
## Intermediate guess of -0.015625.  
## Intermediate guess of 0.0234375.  
## Intermediate guess of 0.00390625.  
## Intermediate guess of -0.005859375.  
## Intermediate guess of -0.0009765625.  
## Intermediate guess of 0.00146484375.  
## Intermediate guess of 0.000244140625.  
## The root of f(x) is at -0.0003662109375.
```

```
g(x) = 3x^3 + 2x - 4
```

```
## g (generic function with 1 method)
```

```
bisection(g, -6, 4)
```

```
## Intermediate guess of -1.0.  
## Intermediate guess of 1.5.  
## Intermediate guess of 0.25.  
## Intermediate guess of 0.875.  
## Intermediate guess of 1.1875.  
## Intermediate guess of 1.03125.  
## Intermediate guess of 0.953125.  
## Intermediate guess of 0.9140625.  
## Intermediate guess of 0.89453125.  
## Intermediate guess of 0.904296875.  
## Intermediate guess of 0.8994140625.  
## Intermediate guess of 0.90185546875.  
## Intermediate guess of 0.900634765625.  
## The root of f(x) is at 0.9012451171875.
```

```
h(x) = cos(x)
```

```
## h (generic function with 1 method)
```

```
bisection(h, -pi, pi)
```

```
## Intermediate guess of 0.0.  
## Intermediate guess of -1.5707963267948966.  
## Intermediate guess of -2.356194490192345.  
## Intermediate guess of -1.9634954084936207.  
## Intermediate guess of -1.7671458676442586.  
## Intermediate guess of -1.6689710972195777.  
## Intermediate guess of -1.6198837120072371.  
## Intermediate guess of -1.595340019401067.  
## Intermediate guess of -1.5830681730979819.  
## Intermediate guess of -1.5769322499464393.  
## Intermediate guess of -1.573864288370668.  
## Intermediate guess of -1.5723303075827824.  
## The root of f(x) is at -1.5715633171888395.
```

# The bisection method

The bisection method works by continually bisecting the interval and only keeping the half interval with the zero until "convergence"

1. Select the midpoint of  $[a, b]$ ,  $(a + b)/2$
2. Zero must be in the lower or upper half
3. Check the sign of the midpoint, if it has the same sign as the lower bound a root must be the right subinterval
4. Select the midpoint of  $[(a + b)/2, b]$ ...

# The bisection method

The bisection method is incredibly robust: if a function  $f$  satisfies the IVT, it is **guaranteed to converge in a specific number of iterations**

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The bisection method is incredibly robust: if a function  $f$  satisfies the IVT, it is **guaranteed to converge in a specific number of iterations**

A root can be calculated to arbitrary precision  $\epsilon$  in a maximum of  $\log([b - a]/\epsilon)/\log(2)$  iterations

Robustness comes with drawbacks:

1. It only works in one dimension
2. It is slow because it only uses information about the function's level

# Function iteration

Fixed points can be computed using function iteration

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**Code up a function iteration problem**

# Function iteration

Function iteration is pretty simple to implement

```
function function_iteration(f, guess)
    tolerance = 1e-3                                # tolerance for solution
    x_old = guess                                    # initialize old x value
    x = 1e-10                                       # initialize current x
    difference = 1e10                                 # initialize bound difference

    @time while abs(difference) > tolerance          # loop until convergence
        println("Intermediate guess of $x.")
        x = f(x_old)                                  # new x = f(old x)
        difference = x - x_old
        x_old = x

    end
    println("The fixed point of f(x) is at $x.")
end;
```

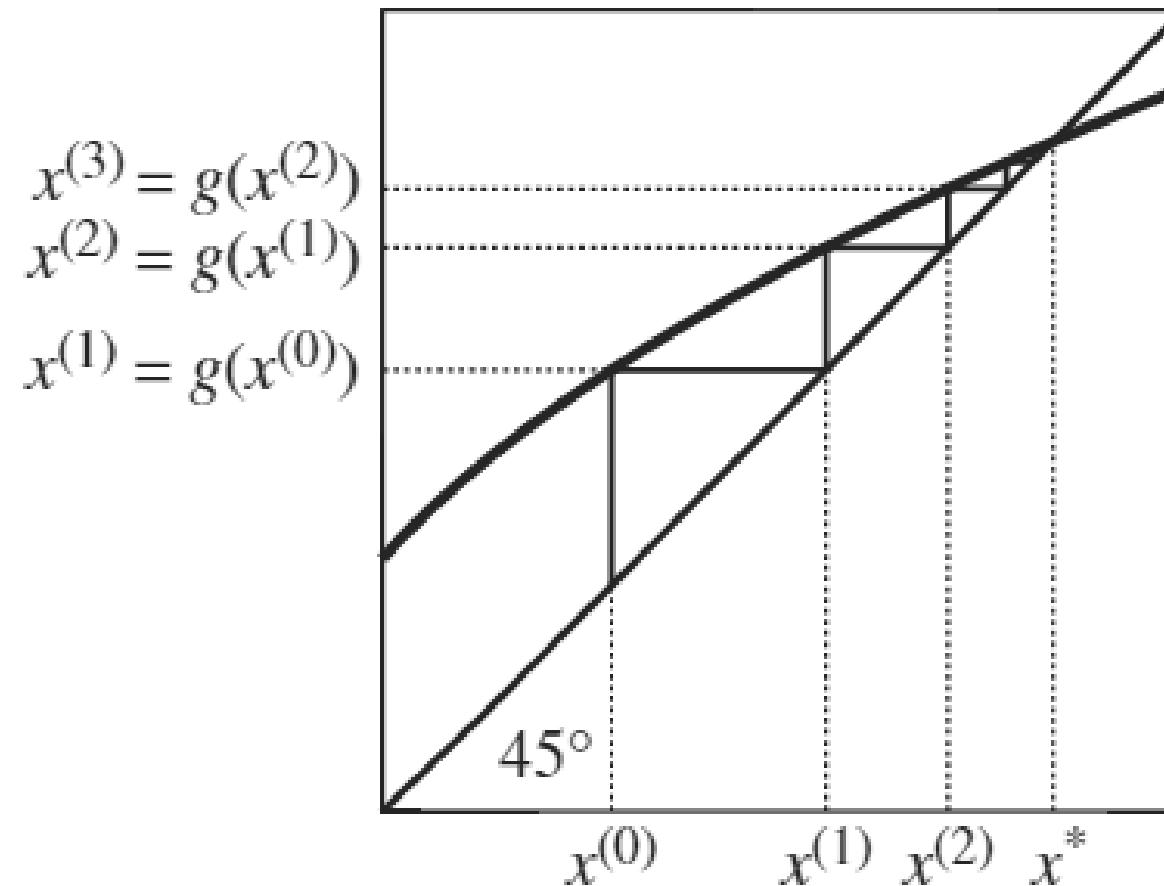
```
f(x) = x^(-0.5)
```

```
## f (generic function with 1 method)
```

```
function_iteration(f, 2.)
```

```
## Intermediate guess of 1.0e-10.  
## Intermediate guess of 0.7071067811865476.  
## Intermediate guess of 1.189207115002721.  
## Intermediate guess of 0.9170040432046712.  
## Intermediate guess of 1.0442737824274138.  
## Intermediate guess of 0.9785720620877002.  
## Intermediate guess of 1.0108892860517005.  
## Intermediate guess of 0.9945994234836332.  
## Intermediate guess of 1.0027112750502025.  
## Intermediate guess of 0.9986471128909702.  
## Intermediate guess of 1.0006771306930664.  
## Intermediate guess of 0.9996616064962437.  
## 0.002017 seconds (924 allocations: 233.763 KiB)  
## The fixed point of f(x) is at 1.0001692397053021.
```

# Function iteration



# Function iteration

Function iteration can be quick, but is not always guaranteed to converge

# Newton's method

Newton's method and variants are the workhorses of solving n-dimensional non-linear problems

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Take a hard non-linear problem and replace it with a sequence of linear problems

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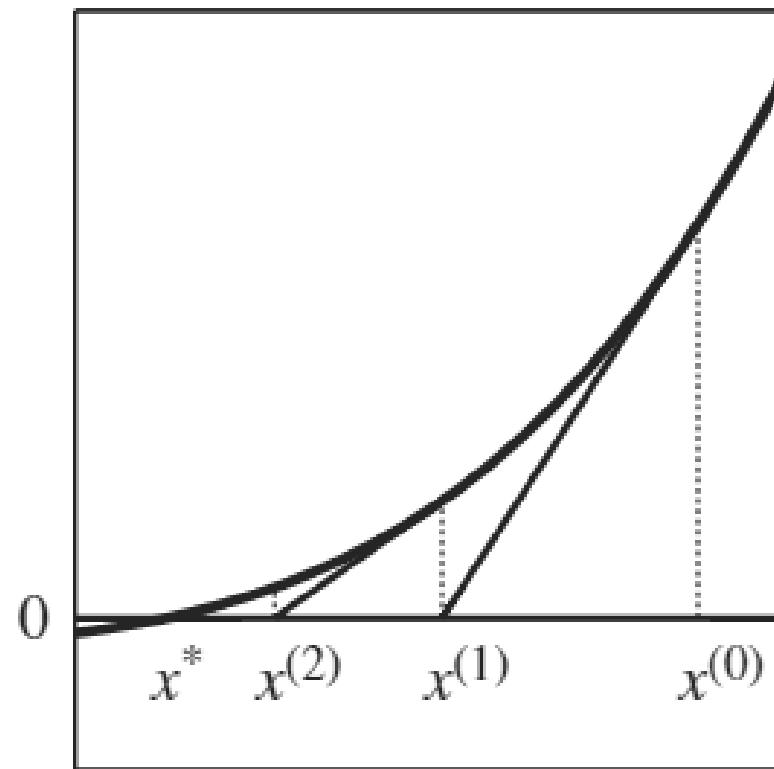
What's the idea?

Take a hard non-linear problem and replace it with a sequence of linear problems

Under certain conditions the sequence of solutions will converge to the true solution

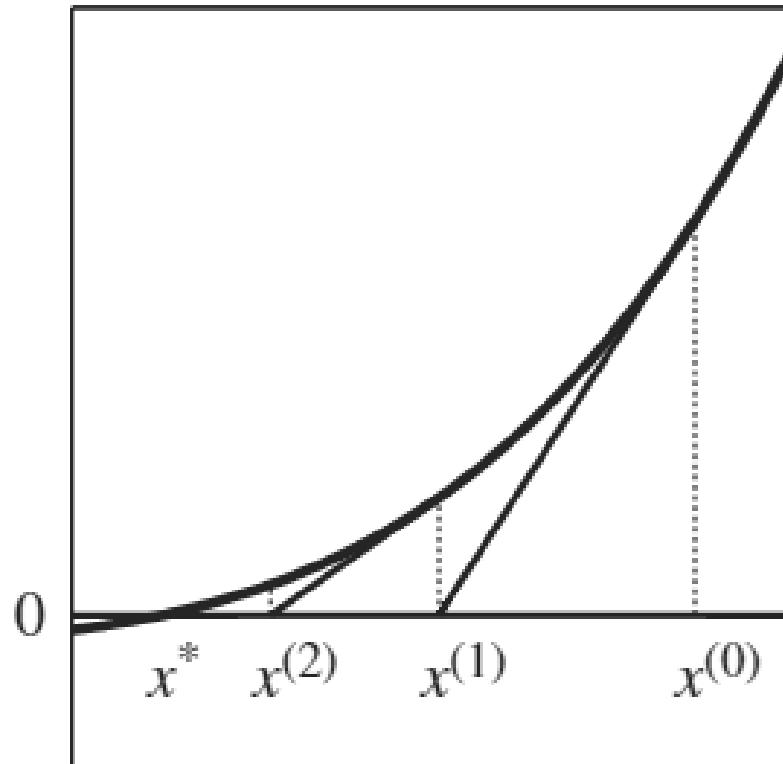
# Newton's method

Here's a graphical depiction of Newton's method:



# Newton's method

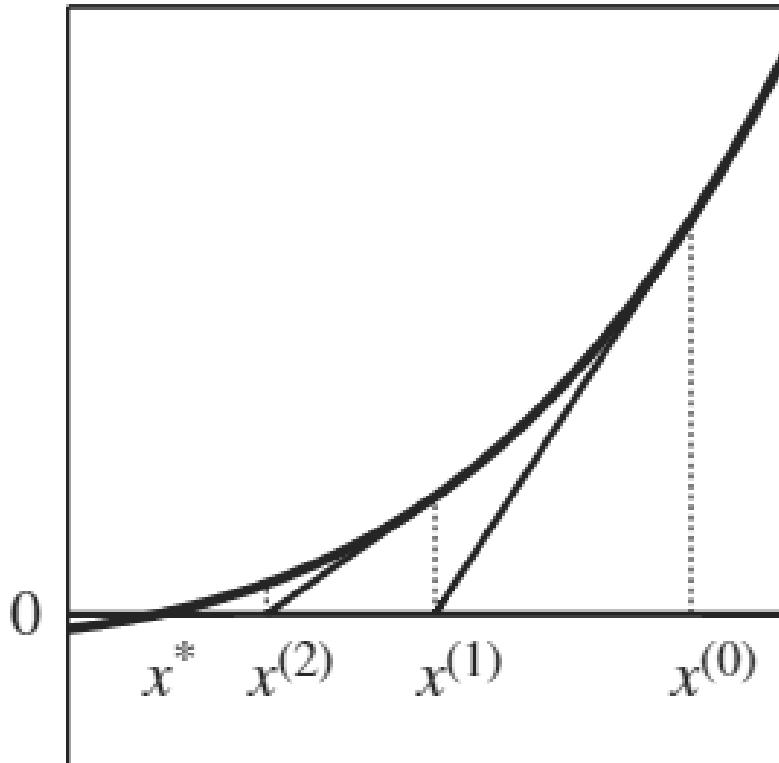
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# Newton's method

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Approximate the non-linear function with its first-order Taylor expansion about  $x^{(0)}$

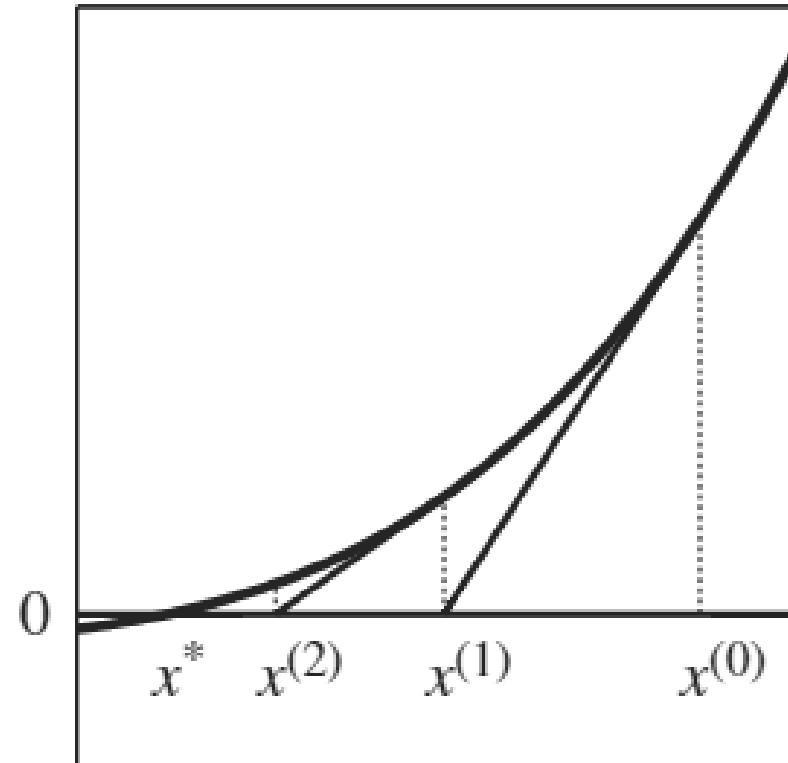


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This is just the tangent line at  $x^0$ , solve for the root of this linear approximation, call it  $x^{(1)}$



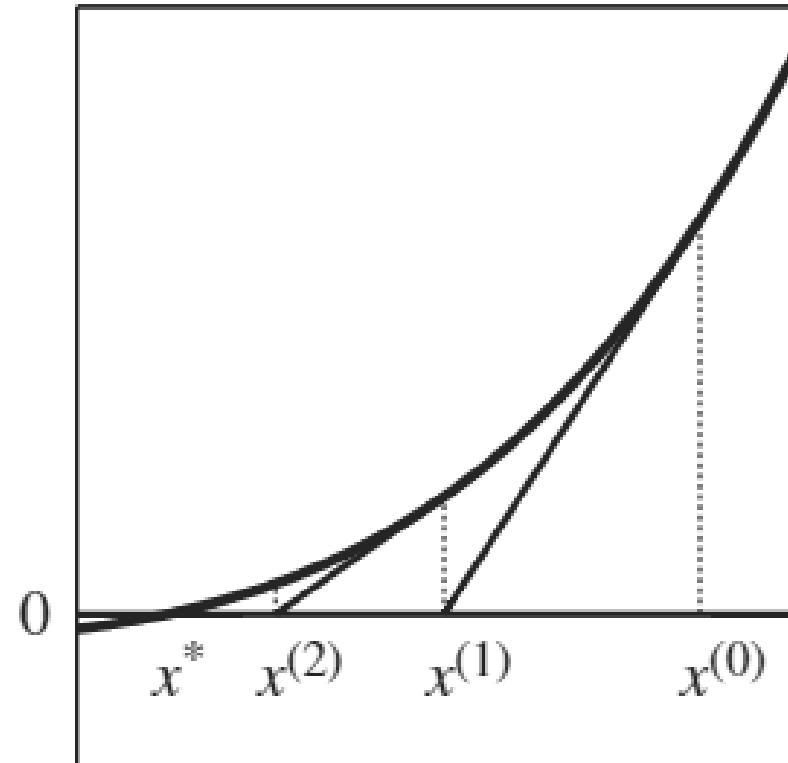
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Repeat starting at  $x^{(1)}$



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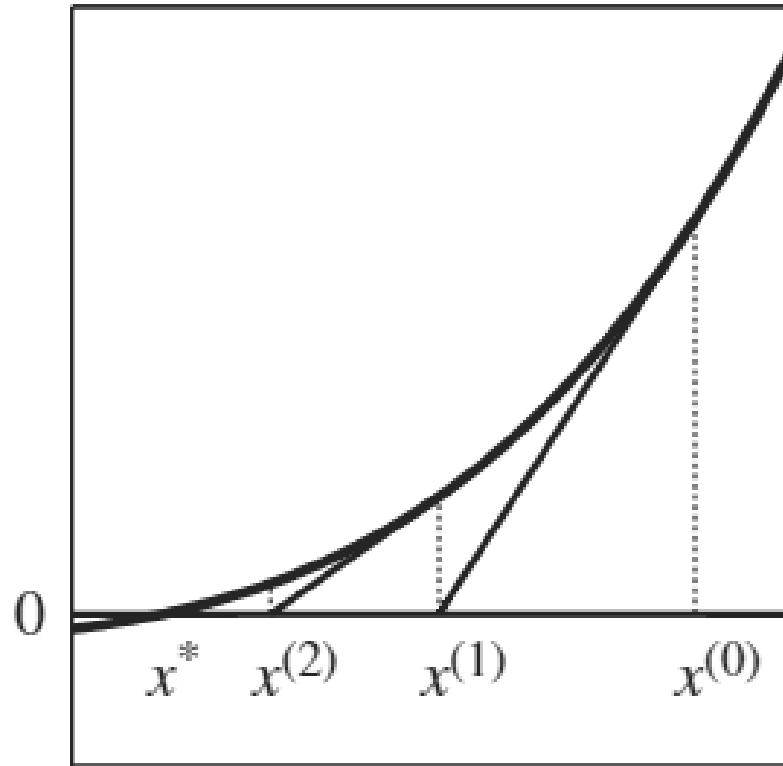
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Repeat starting at  $x^{(1)}$

This can be applied to a function with an arbitrary number of dimensions



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Begin with some initial guess of the root vector  $\mathbf{x}^{(0)}$

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Our new guess  $\mathbf{x}^{(k+1)}$  given some arbitrary point in the algorithm,  $\mathbf{x}^{(k)}$ , is obtained by approximating  $f(\mathbf{x})$  using a first-order Taylor expansion about  $\mathbf{x}^{(k)}$  and solving for  $\mathbf{x}$ :

$$\begin{aligned} f(\mathbf{x}) &\approx f(\mathbf{x}^{(k)}) + f'(\mathbf{x}^{(k)})(\mathbf{x} - \mathbf{x}^{(k)}) = 0 \\ \Rightarrow \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} - [f'(\mathbf{x}^{(k)})]^{-1} f(\mathbf{x}^{(k)}) \end{aligned}$$

# Newton's method

**Code up Newton's method**

# Newton's method

## Code up Newton's method

```
function newtons_method(f, f_prime, guess)
    diff = Inf      # Initialize problem
    tol = 1e-5
    x_old = guess
    x = 1e10

    while abs(diff) > tol
        x = f(x_old) - f(x_old)/f_prime(x_old) # Root of linear approximation
        diff = x - x_old
        x_old = x
    end
    println("The root of f(x) is at $x.")
end;
```

# Newton's method

```
f(x) = x^3;  
f_prime(x) = 3x^2;  
newtons_method(f, f_prime, 1.)
```

```
## The root of f(x) is at 1.231347218094855e-6.
```

# Newton's method

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f(x) = x^3;  
f_prime(x) = 3x^2;  
newtons_method(f, f_prime, 1.)
```

## The root of  $f(x)$  is at 1.231347218094855e-6.

```
f(x) = sin(x);  
f_prime(x) = cos(x);  
newtons_method(f, f_prime, pi/4)
```

## The root of  $f(x)$  is at 5.941936124988917e-19.

# Newton's method

Newton's method has nice properties regarding convergence and speed:

If  $f(x)$  is continuously differentiable, the initial guess is "sufficiently close" to the root, and  $f'(x)$  is invertible near the root, then Newton's method converges to the root

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We need  $f(x)$  to be invertible so the algorithm above is well defined

If  $f'(x)$  is ill-conditioned we can run into problems with rounding error

# Quasi-Newton: Secant method

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2. Can actually be slower to evaluate than finite differences for a nonlinear problem,  
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Using our current root guess  $x^{(k)}$  and our previous root guess  $x^{(k-1)}$ :

$$f'(x^{(k)}) \approx \frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$$

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$$x^{(k+1)} = x^{(k)} - \frac{x^{(k)} - x^{(k-1)}}{f(x^{(k)}) - f(x^{(k-1)})} f(x^{(k)})$$

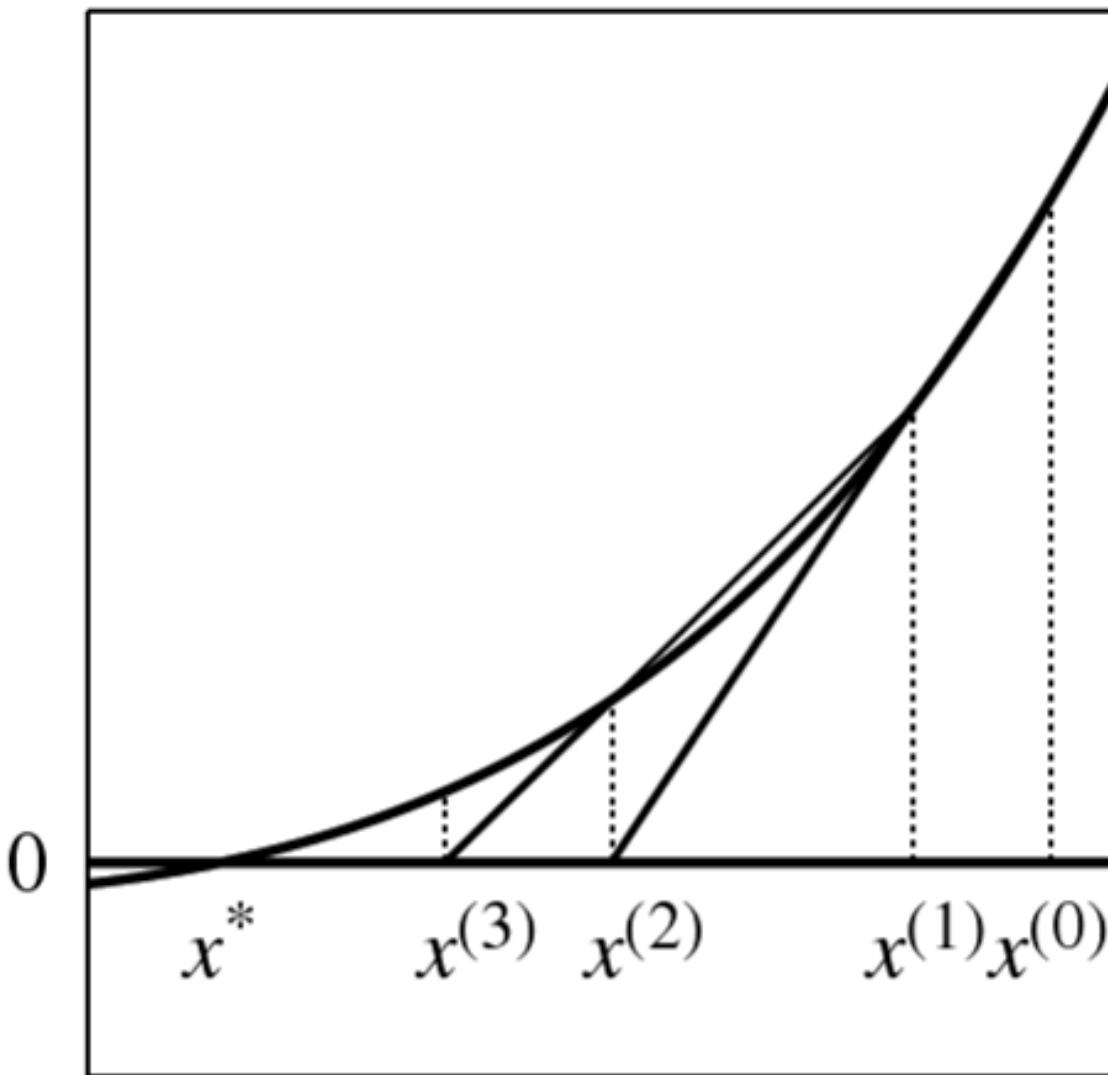
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Now we require two initial guesses so that we have an initial approximation of the derivative

# Quasi-Newton: Secant method



# Quasi-Newton: Broyden's method

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It is a generalization of the secant method where have a sequence of guesses of the Jacobian at the root

We must initially provide a guess of the root,  $x^{(0)}$ , but also a guess of the Jacobian,  $A_{(0)}$

# Quasi-Newton: Broyden's method

Root guess update is the same as before but with our guess of the Jacobian substituted in for the actual Jacobian or the finite difference approximation

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - A_{(k)}^{-1} f(\mathbf{x}^{(k)}).$$

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we still need to update  $A_{(k)}$ : we do this update is performed by making the smallest change, in terms of the Frobenius matrix norm, that satisfies what is called the *secant condition* (under determined if  $n > 1$ ):  $f(\mathbf{x}^{(k+1)}) - f(\mathbf{x}^{(k)}) = A_{(k+1)} (\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)})$

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The updated differences in root guesses, and the function value at those root guesses, should align with our estimate of the Jacobian at that point

# Quasi-Newton: Broyden's method

Root guess update is the same as before but with our guess of the Jacobian substituted in for the actual Jacobian or the finite difference approximation

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - A_{(k)}^{-1} f(\mathbf{x}^{(k)}).$$

we still need to update  $A_{(k)}$ : we do this update is performed by making the smallest change, in terms of the Frobenius matrix norm, that satisfies what is called the *secant condition* (under determined if  $n > 1$ ):  $f(\mathbf{x}^{(k+1)}) - f(\mathbf{x}^{(k)}) = A_{(k+1)} (\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)})$

The updated differences in root guesses, and the function value at those root guesses, should align with our estimate of the Jacobian at that point

$$A_{(k+1)} = A_{(k)} + [f(\mathbf{x}^{(k+1)}) - f(\mathbf{x}^{(k)}) - A_{(k+1)} (\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)})] \frac{\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}}{(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)})^T (\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)})}$$

# Accelerating Broyden

Why update the Jacobian and then invert when we can just update an inverted Jacobian  
 $B = A^{-1}$

$$B_{(k+1)} = B_{(k)} + \frac{[d^{(k)} - u^{(k)}] d^{(k)T} B_{(k)}}{d^{(k)T} u^{(k)}}$$

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Broyden converges under relatively weak conditions:

1.  $f$  is continuously differentiable,
2.  $\mathbf{x}^{(0)}$  is close to the root of  $f$
3.  $f'$  is invertible around the root
4.  $A_0$  is sufficiently close to the Jacobian

# Convergence speed

Rootfinding algorithms will converge at different speeds in terms of the number of operations

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A sequence of iterates  $x^{(k)}$  is said to converge to  $x^*$  at a rate of order  $p$  if there is a constant  $C$  such that

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for sufficiently large  $k$

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for sufficiently large  $k$

If  $C < 1$  and  $p = 1$ , the rate of convergence is linear

If  $1 < p < 2$ , convergence is superlinear, and if  $p = 2$  convergence is quadratic. The higher order the convergence rate, the faster it converges

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- Newton:  $p = 2$

# Convergence speed

Convergence rates only account for the number of **iterations** of the method

The steps taken in a given iteration of each solution method may vary in computational cost because of differences in the number of arithmetic operations

Although an algorithm may take more iterations to solve,  
each iteration may be solved faster and the overall algorithm takes less time

# Convergence speed

Ex:

- Bisection method only requires a single function evaluation during each iteration
- Function iteration only requires a single function evaluation during each iteration
- Broyden's method requires both a function evaluation and matrix multiplication
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Bisection and function iteration are usually slow

Broyden's method can be faster than Newton's method if derivatives are costly to compute

# Convergence speed

Consider an example where  $f(x) = x - \sqrt{x} = 0$

What does convergence look like across our main approaches in terms of the  $L^1$ -norm if all guesses start at  $x^{(0)} = 0.5$ ?

$k$	Function Iteration	Broyden's Method	Newton's Method
1	2.9e-001	-2.1e-001	-2.1e-001
2	1.6e-001	3.6e-002	-8.1e-003
3	8.3e-002	1.7e-003	-1.6e-005
4	4.2e-002	-1.5e-005	-6.7e-011
5	2.1e-002	6.3e-009	0.0e+000
6	1.1e-002	2.4e-014	0.0e+000
7	5.4e-003	0.0e+000	0.0e+000
8	2.7e-003	0.0e+000	0.0e+000
9	1.4e-003	0.0e+000	0.0e+000
10	6.8e-004	0.0e+000	0.0e+000
15	2.1e-005	0.0e+000	0.0e+000
20	6.6e-007	0.0e+000	0.0e+000
25	2.1e-008	0.0e+000	0.0e+000

# Complementarity problems: rootfinding

Let:

- $x$  be an n-dimensional vector of some economic action
- $a_i$  denotes a lower bound on action  $i$ , and  $b_i$  denotes the upper bound on action  $i$
- $f_i(x)$  denotes the marginal arbitrage profit of action  $i$

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- $f_i(x)$  denotes the marginal arbitrage profit of action  $i$

There are disequilibrium profit opportunities if

1.  $x_i < b_i$  and  $f_i(x) > 0$  (here we can increase profits by raising  $x_i$ )
2.  $x_i > a_i$  and  $f_i(x) < 0$  (we can increase profits by decreasing  $x_i$ )

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We obtain a no-arbitrage equilibrium if and only if  $x$  solves the complementary problem  $CP(f, a, b)$

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We can write out the problem as finding a vector  $x \in [a, b]$  that solves

$$x_i > a_i \Rightarrow f_i(x) \geq 0 \quad \forall i = 1, \dots, n$$

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At interior solution, the function be precisely be zero

Corner solution at the upper bound  $b_i$  for  $x_i \rightarrow f$  must be increasing in direction  $i$

The opposite is true if we are at the lower bound

# Complementarity problems

Economic problems are complementarity problems where we are finding a root of a function (e.g. marginal profit) subject to some constraint (e.g. price floors)

The Karush-Kuhn-Tucker theorem shows that  $x$  solves the constrained optimization problem if and only if it solves the complementarity problem

# Complementarity problems

**Example:** single commodity competitive spatial price equilibrium model

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- excess demand for the commodity in region  $i$  is  $E_i(p_i)$

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Trade between regions has marginal transportation cost between regions  $i$  and  $j$  of  $c_{ij}$

- $x_{ij}$ : the amount of the good shipped from region  $i$  to region  $j$
- capacity constraint:  $b_{ij}$

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At an equilibrium only if all the arbitrage opportunities are gone: for all region pairs  $i$  and  $j$

$$0 \leq x_{ij} \leq b_{ij}$$

$$x_{ij} > 0 \Rightarrow p_j - p_i - c_{ij} \geq 0$$

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Market clearing in each region  $i$  requires that net imports = excess demand

$$\sum_k [x_{ki} - x_{ik}] = E_i(p_i)$$

This implies that we can solve for the price in region  $i$ ,

$$p_i = E_i^{-1} \left( \sum_k [x_{ki} - x_{ik}] \right)$$

# Complementarity problems

Finally, if we define marginal arbitrage profit from shipping another unit from  $i$  to  $j$  as

$$f_{ij}(x) = E_j^{-1} \left( \sum_k [x_{kj} - x_{jk}] \right) - E_i^{-1} \left( \sum_k [x_{ki} - x_{ik}] \right) - c_{ij}$$

then  $x$  is an equilibrium vector of trade flows if and only if  $x$  solves  $CP(f, 0, b)$  and  $x, f$ , and  $b$  are  $n^2 \times 1$  vectors

Even this complex trade-equilibrium model can be reduced to a simple complementarity problem

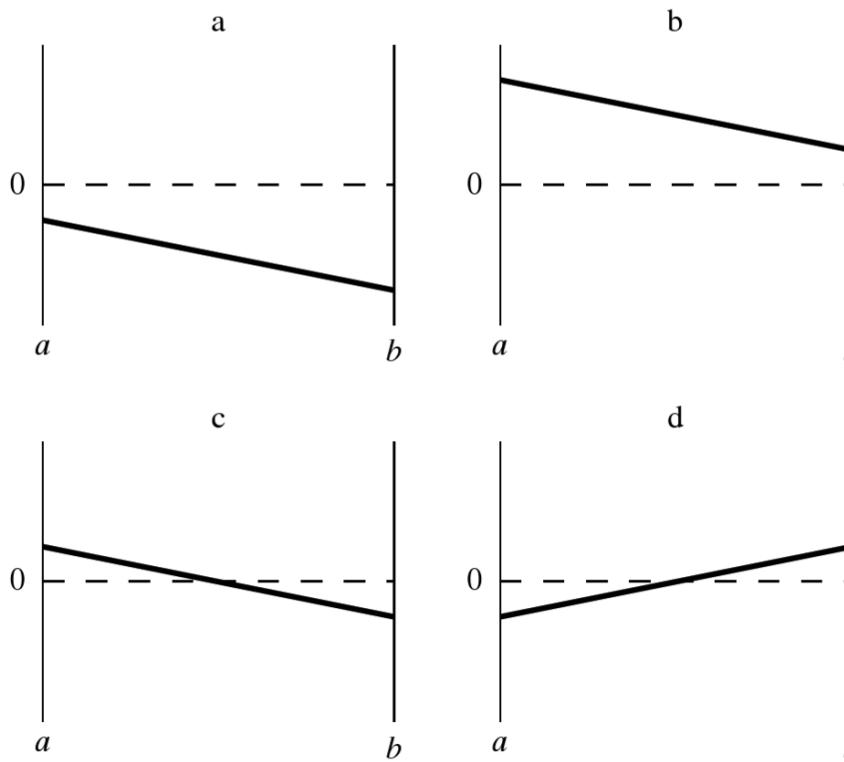
# Complementarity problems

Decentralized models can generally be solved by reducing them to complementarity problems, e.g:

1. Competitive energy markets with cross-market cap and trade or capacity constraints
2. Federalism models
3. etc etc

# Complementarity problems

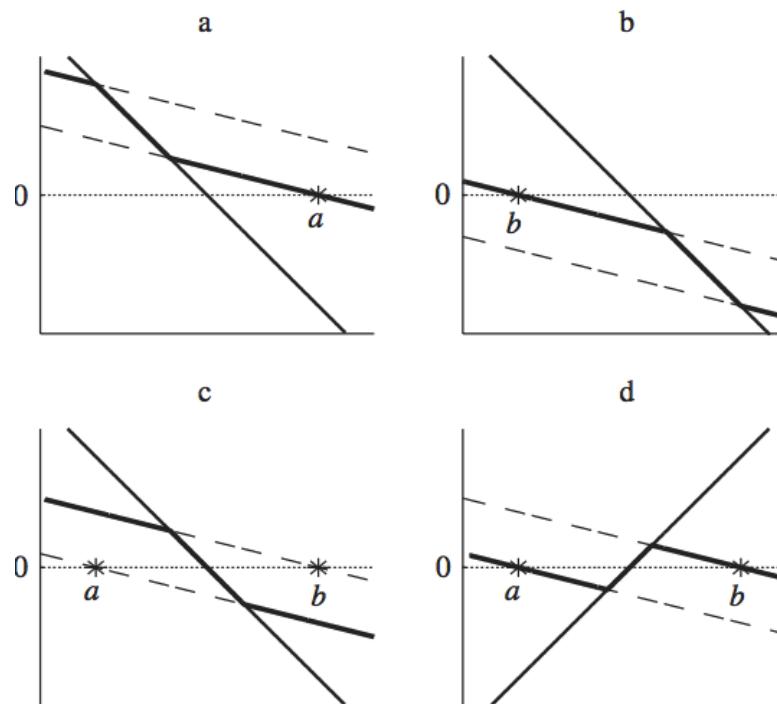
Four plots of marginal arbitrage profit  $f_i(x)$ , what is the equilibrium choice of  $x$ ?



# How do we solve them?

A complementarity problem  $CP(f, a, b)$  can be re-framed as a rootfinding problem easily

$$\hat{f}(x) = \min(\max(f(x), a - x), b - x) = 0$$



# How do we solve them?

We can then solve the problem with conventional rootfinding techniques or approximate this with a smooth function to make it easier on a rootfinder

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The workhorse solver for complementarity problems is the PATH solver: Julia wrapper can be found [here](#)

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**Derivative-using vs derivative-free:** Do we want to use higher-order information?

# Maximization (minimization) methods

I'll focus on local solvers, common global solvers I won't cover:

1. Genetic algorithms
2. Simulated annealing
3. DIRECT
4. Sto-go

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Replace the endpoint of the interval next to the evaluated point with the highest value  
→ keep the lower evaluated point in the interval → guarantees that a local minimum still exists

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There's one algorithm that satisfies this

# Derivative free optimization: Golden search

Golden search algorithm for point selection:

$$x_i = a + \alpha_i(b - a)$$
$$\alpha_1 = \frac{3 - \sqrt{5}}{2} \quad \alpha_2 = \frac{\sqrt{5} - 1}{2}$$

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**Write out a golden search algorithm**

# Golden search

```
function golden_search(f, lower_bound, upper_bound)
    alpha_1 = (3 - sqrt(5))/2 # GS parameter 1
    alpha_2 = (sqrt(5) - 1)/2 # GS parameter 2
    tolerance = 1e-2          # tolerance for convergence
    difference = 1e10
    while difference > tolerance
        x_1 = lower_bound + alpha_1*(upper_bound - lower_bound) # new x_1
        x_2 = lower_bound + alpha_2*(upper_bound - lower_bound) # new x_2
        if f(x_1) < f(x_2)      # reset bounds
            upper_bound = x_2
        else
            lower_bound = x_1
        end
        difference = x_2 - x_1
    end
    println("Minimum is at x = $((lower_bound+upper_bound)/2).")
end;
```

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    end
    println("Minimum is at x = $((lower_bound+upper_bound)/2).")
end;
```

```
f(x) = 2x^2 + 9x;
golden_search(f, -10, 10)
```

```
## Minimum is at x = -2.2483173872886444.
```

# Nelder-Mead: Simplex

Golden search is nice and simple but only works in one dimension

There are several derivative free methods for minimization that work in multiple dimensions, the most commonly used one is **Nelder-Mead (NM)**

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NM works by first constructing a simplex: we evaluate the function at  $n + 1$  points in an  $n$  dimensional problem

It then manipulates the highest value point, similar to golden search

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- **Centroid:** calculate  $x_0$ , the centroid of the non -  $x_{n+1}$  points
- **Reflection:** reflect  $x_{n+1}$  through the opposite face of the simplex and evaluate the new point:  $x_r = x_0 + \alpha(x_0 - x_{n+1})$ ,  $\alpha > 0$ 
  - If this improves upon the second-highest (e.g. its lower) but is not the lowest value point, replace  $x_{n+1}$  with  $x_r$  and restart
  - If this is the lowest value point so far, go to step 4
  - If  $f(x_r) > f(x_n)$  go to step 5

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- **Expansion:** push the reflected point further in the same direction
- **Contract:** Contract the highest value point toward the middle
  - Compute  $x_c = x_0 + \gamma(x_0 - x_{n+1})$ ,  $0 < \gamma \leq 0.5$
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  - Else go to step 6

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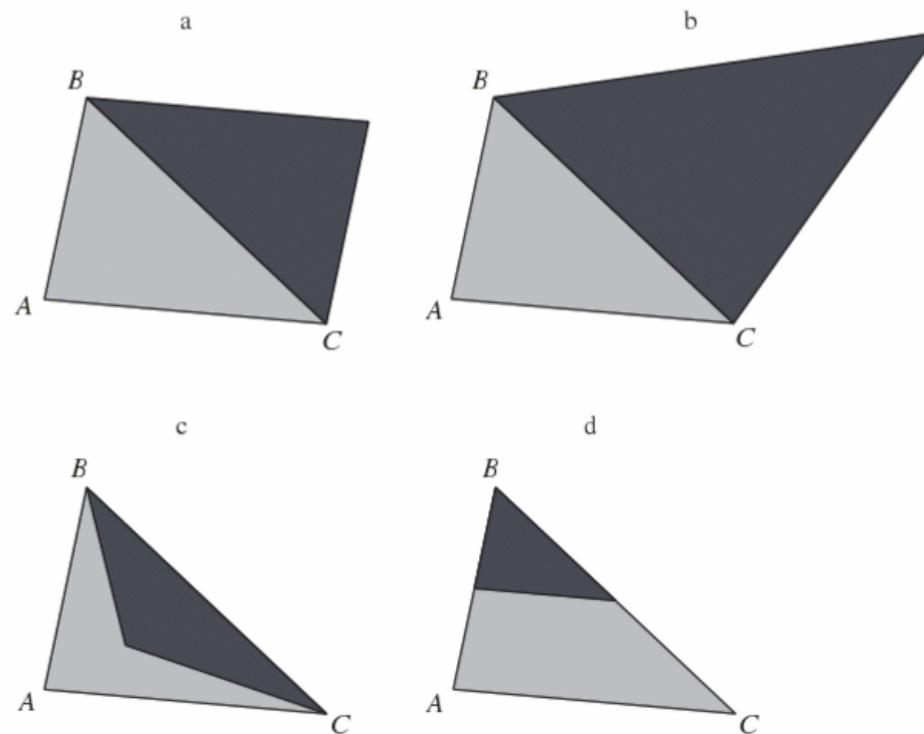
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- **Shrink:** shrink the simplex toward the best point
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Nelder-Mead is a pain to code efficiently (i.e. don't spend the time doing it yourself) but is in the `Optim.jl` package

# Nelder-Mead: Simplex



Nelder-Mead is commonly used but slow and unreliable, no real useful convergence properties, avoid using it

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Typically analytical problems are set up to have a unique minimum so any local solver can generally find the global optimum

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How do we find a local minimum?

Do we need to evaluate every single point?

# The general unconstrained approach

Optimization algorithms typically have the following set up:

1. Start at some  $x_0$
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If  $f$  is twice continuously differentiable, we can use the gradient  $\nabla f$  and Hessian  $\nabla^2 f$  to figure out if  $x^*$  is a local minimizer

# The general unconstrained approach

Taylor's Theorem tells us that if  $f$  is twice differentiable, then there exists a  $t \in (0, 1)$  such that

$$f(x^* + p) = f(x^*) + \nabla f(x^*)^T p + \frac{1}{2!} p^T \nabla^2 f(x^* + tp) p$$

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From here we can prove the usual necessary and sufficient conditions for a local optimum

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Most modern optimization problems fall into one of two classes:

1. Line search
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The relationship between these two approaches has a lot of similarities  
to the relationship between the constrained problem and the dual Lagrange problem

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We are finding the distance to move,  $\alpha$  in direction  $p_k$  that minimizes our objective  $f$

# Line search algorithms

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

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

# Line search: direction choice

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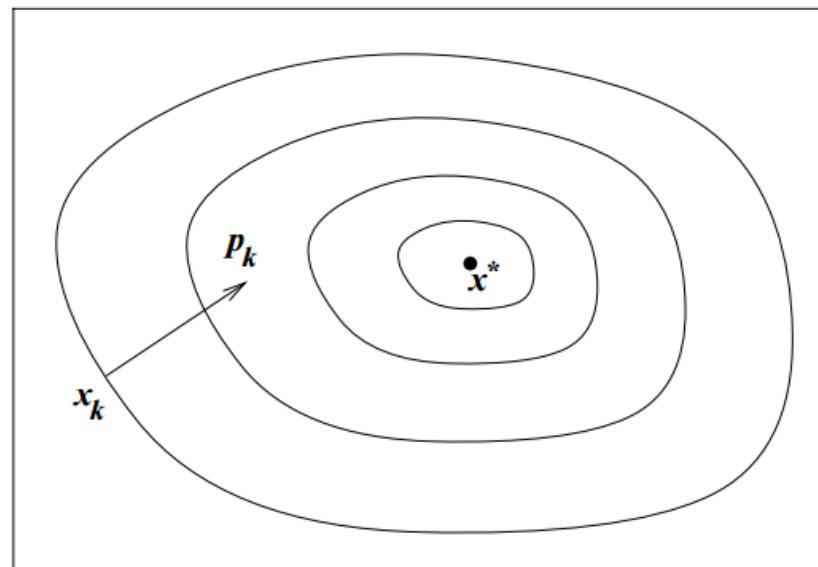
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The rate of change in  $f$  along  $p$  at  $x_k$  ( $\alpha = 0$ ) is  $p^T \nabla f_k$

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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  $-\nabla f_k$

# Line search: steepest descent

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

It may select the step length  $\alpha_k$  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

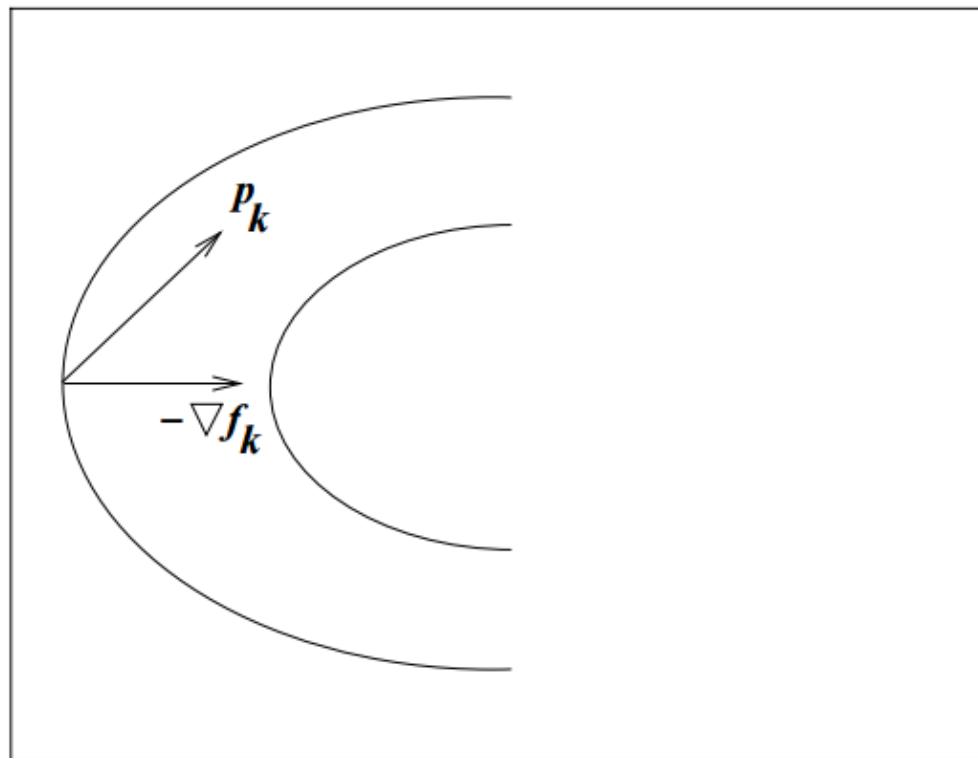
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Any descent direction, i.e. one that is within  $45^\circ$  of  $-\nabla f_k$ ,  
is guaranteed to produce a decrease in  $f$  as long as the step size is sufficiently small



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**Is  $-\nabla f_k$  always the best search direction?**

# Newton's method

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Newton's direction comes out of the second order Taylor series approximation to  
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We find the Newton direction by selecting the vector  $p$  that minimizes  $f(x_k + p)$

This ends up being

$$p_k^N = -\frac{\nabla f_k}{\nabla^2 f_k}$$

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**Drawback:** requires explicit computation of the Hessian,  $\nabla^2 f(x)$

- Quasi-Newton solvers also exist (e.g. BFGS, L-BFGS, etc)

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**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**

# Trust region methods

Trust region problems can be formulated as

$$\min_p m_k(x_k + p)$$

where

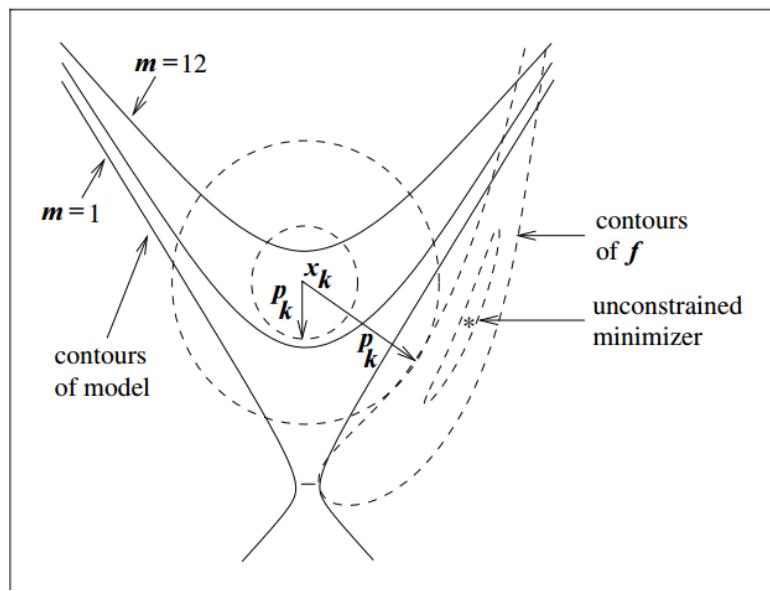
- $x_k + p \in \Gamma$
- $\Gamma$  is a ball defined by  $\|p\|_2 \leq \Delta$
- $\Delta$  is called the trust region radius

# 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



# Line search vs trust region

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Line search first picks a direction then searches along that direction for the optimal step length

Trust region first defines our step length via the trust region radius, then searches for the optimal direction

# Line search vs trust region

There is a special case of the trust region where if we set  $B_k$ , the approximate Hessian, to zero, the solution to the problem is

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

This is just the steepest descent solution for the line search problem

# Problem scaling

The **scaling** of a problem matters for optimization performance

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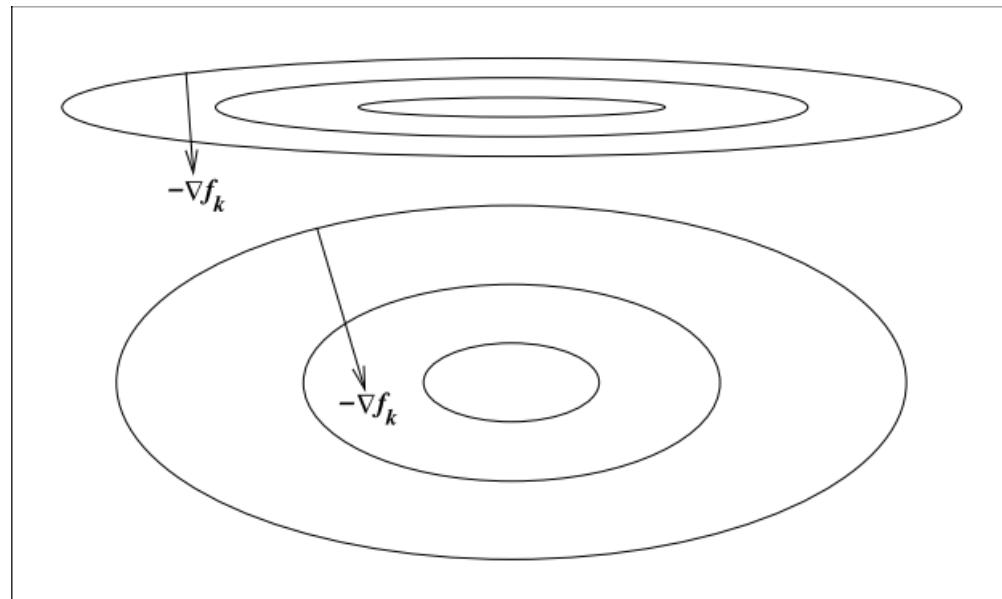
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How do we solve this issue?

Rescale the problem: put them in units that are generally within an order of magnitude of 1

- Investment rate in percentage terms: 0% – 100%
- Consumption in units of trillion dollars instead of dollars

# Constrained optimization

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We will discuss three types of constrained optimization algorithms

- Penalty methods
- Active set methods
- Interior point methods

# Constrained optimization

These are the algorithms in workhorse commercial solvers: KNITRO

## Algorithms description

This section only describes the four algorithms implemented in Knitro in very broad terms. For details, please see the [Bibliography](#).

- Interior/Direct algorithm

Interior-point methods (also known as barrier methods) replace the nonlinear programming problem by a series of barrier subproblems controlled by a barrier parameter. Interior-point methods perform one or more minimization steps on each barrier subproblem, then decrease the barrier parameter and repeat the process until the original problem has been solved to the desired accuracy. The Interior/Direct method computes new iterates by solving the primal-dual KKT matrix using direct linear algebra. The method may temporarily switch to the Interior/CG algorithm, described below, if it encounters difficulties.

- Interior/CG algorithm

This method is similar to the Interior/Direct algorithm. It differs mainly in the fact that the primal-dual KKT system is solved using a projected conjugate gradient iteration. This approach differs from most interior-point methods proposed in the literature. A projection matrix is factorized and the conjugate gradient method is applied to approximately minimize a quadratic model of the barrier problem. The use of conjugate gradients on large-scale problems allows Knitro to utilize exact second derivatives without explicitly forming or storing the Hessian matrix. An incomplete Cholesky preconditioner can be computed and applied during the conjugate gradient iterations for problems with equality and inequality constraints. This generally results in improved performances in terms of number of conjugate gradient iterations and CPU time.

# Constrained optimization

These are the algorithms in workhorse commercial solvers: KNITRO

- Active Set algorithm

Active set methods solve a sequence of subproblems based on a quadratic model of the original problem. In contrast with interior-point methods, the algorithm seeks active inequalities and follows a more exterior path to the solution. Knitro implements a sequential linear-quadratic programming (SLQP) algorithm, similar in nature to a sequential quadratic programming method but using linear programming subproblems to estimate the active set. This method may be preferable to interior-point algorithms when a good initial point can be provided; for example, when solving a sequence of related problems. Knitro can also "crossover" from an interior-point method and apply Active Set to provide highly accurate active set and sensitivity information.

- Sequential Quadratic Programming (SQP) algorithm

The SQP method in Knitro is an active-set method that solves a sequence of quadratic programming (QP) subproblems to solve the problem. This method is primarily designed for small to medium scale problems with expensive function evaluations – for example, problems where the function evaluations involve performing expensive black-box simulations and/or derivatives are computed via finite-differencing. The SQP iteration is expensive since it involves solving a QP subproblem. However, it often converges in the fewest number of function/gradient evaluations, which is why this method is often preferable for situations where the evaluations are the dominant cost of solving the model.

# Constrained optimization

These are the algorithms in workhorse commercial solvers: fmincon/MATLAB

All Algorithms	
Algorithm	<p>Choose the optimization algorithm:</p> <ul style="list-style-type: none"><li>• 'interior-point' (default)</li><li>• 'trust-region-reflective'</li><li>• 'sqp'</li><li>• 'sqp-legacy' (optimoptions only)</li><li>• 'active-set'</li></ul> <p>For information on choosing the algorithm, see <a href="#">Choosing the Algorithm</a>.</p> <p>The trust-region-reflective algorithm requires:</p> <ul style="list-style-type: none"><li>• A gradient to be supplied in the objective function</li><li>• Specify <code>ObjectiveGradient</code> to be set to <code>true</code></li><li>• Either bound constraints or linear equality constraints, but not both</li></ul> <p>If you select the 'trust-region-reflective' algorithm and these conditions are not all satisfied, fmincon throws an error.</p> <p>The 'active-set', 'sqp-legacy', and 'sqp' algorithms are not large-scale. See <a href="#">Large-Scale vs. Medium-Scale Algorithms</a>.</p>

# Constrained optimization: Penalty methods

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One way is to introduce a **penalty function** into our objective and remove the constraint:

$$Q(x; \mu) = f(x) + \frac{\mu}{2} \sum_i c_i^2(x)$$

where  $\mu$  is the penalty parameter

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There are also augmented Lagrangian methods that take the quadratic penalty method and add in explicit estimates of Lagrange multipliers to help force binding constraints to bind precisely

# Constrained optimization: Penalty method example

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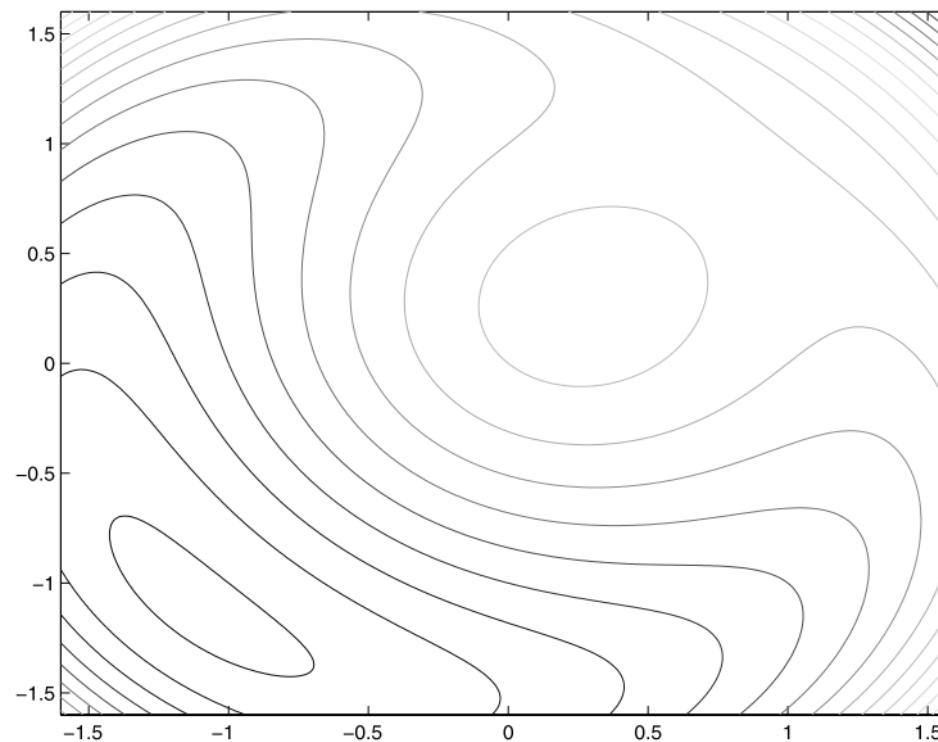
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Let's ramp up  $\mu$  and see what happens to how the function looks

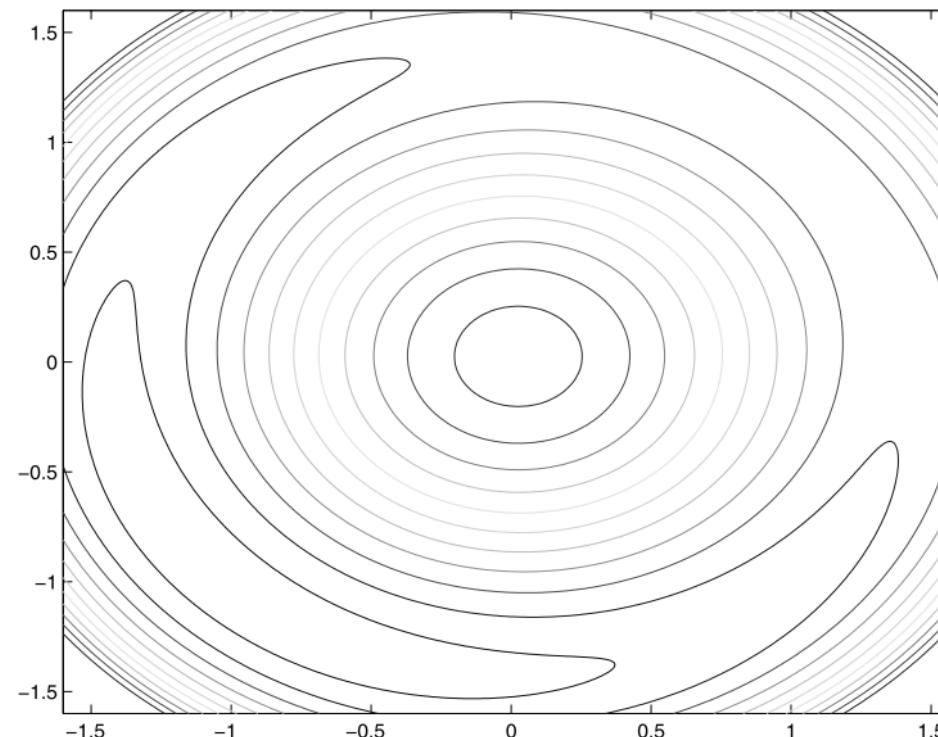
# Constrained optimization: Penalty method example

$\mu = 1$ , solution is around  $(-1.1, -1.1)$



# Constrained optimization: Penalty method example

$\mu = 10$ , solution is very close to  $(-1, -1)$ , can easily see trough, and rapid value increase outside  $x_1^2 + x_2^2 = 2$



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Denote  $A(x)^T$  as the Jacobian of the constraints

$$A(x)^T = [\nabla c_1(x), \dots, \nabla c_m(x)]$$

# Constrained optimization: Active set methods

The first-order conditions  $F(x, \lambda)$  can be written as,

$$\begin{aligned}\nabla f(x) - A(x)^T \lambda &= 0 \\ c(x) &= 0\end{aligned}$$

Any solution to the equality constrained problem, where  $A(x^*)$  has full rank also satisfies the first-order necessary conditions

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Active set methods use Newton's method to find the solution  $(x^*, \lambda^*)$  of  $F(x, \lambda)$

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**Main idea:** recognize that if an inequality constraint is not binding, or **active**, then it has no influence on the solution

→ in the iteration procedure we can effectively ignore it

Active set methods find ways to reduce the complexity of the optimization routine by selectively ignoring constraints that are not active (i.e. non-positive Lagrange multipliers) or close to being active

# Constrained optimization: Interior point methods

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The name **interior point** comes from the algorithm traversing the domain along the interior of the inequality constraints

**Issue:** how do we ensure we are on the interior of the feasible set?

**Main idea:** impose a **barrier** to stop the solver from letting a constraint bind

# Constrained optimization: Interior point methods

Consider the following constrained optimization problem

$$\begin{aligned} & \min_x f(x) \\ \text{subject to: } & c_E(x) = 0, c_I(x) \geq 0 \end{aligned}$$

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Reformulate this problem as

$$\begin{aligned} & \min_{x,s} f(x) \\ \text{subject to: } & c_E(x) = 0, c_I(x) - s = 0, s \geq 0 \end{aligned}$$

where  $s$  is a vector of slack variables for the constraints

# Constrained optimization: Interior point methods

Final step: introduce a **barrier function** to eliminate the inequality constraint,

$$\min_{x,s} f(x) - \mu \sum_{i=1}^m \log(s_i)$$

$$\text{subject to: } c_E(x) = 0, c_I(x) - s = 0$$

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The solution to the barrier problem converges to that of the original problem

# Best practices for optimization

Plug in your guess, let the solver go, and you're done right?

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These algorithms are not guaranteed to always find even a local solution, you need to test and make sure you are converging correctly

# Check exitflags: KNITRO-specific numbers here

Exitflags tell you why the solver stopped, exit flags of 0 or -10X are generally good, anything else is bad

-10X can indicate bad scaling, ill-conditioning, etc

Value	Description
0	Locally optimal solution found.
-100	Current feasible solution estimate cannot be improved. Nearly optimal.
-101	Relative change in feasible solution estimate < xtol.
-102	Current feasible solution estimate cannot be improved.
-103	Relative change in feasible objective < ftol for ftol_iters.
-200	Convergence to an infeasible point. Problem may be locally infeasible.
-201	Relative change in infeasible solution estimate < xtol.
-202	Current infeasible solution estimate cannot be improved.
-203	Multistart: No primal feasible point found.
-204	Problem determined to be infeasible with respect to constraint bounds.
-205	Problem determined to be infeasible with respect to variable bounds.
-300	Problem appears to be unbounded.

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Interior-point is usually the default in constrained optimization solvers (low memory usage, fast), but try other algorithms and see if the solution generally remains the same

# Be aware of tolerances

Two main tolerances in optimization:

1. `ftol` is the tolerance for the change in the function value (absolute and relative)
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It depends

Explore sensitivity to tolerance, typically pick a conservative (small) number

- Defaults in solvers are usually `1e-6`

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(e.g. so your big MLE converges)

Issue is that  $1e-3$  might be pretty big for your problem  
if you haven't checked that your solution is not sensitive to the tolerance

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Bad ones can give you terrible performance, or wrong answers if your problem isn't perfect

- e.g. bad scaling, not well-conditioned, multiple equilibria