SciencesPo Computational Economics
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Florian Oswald

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1 Optimization 2: Algorithms and Constraints

Florian Oswald Sciences Po, 2018

1.1 Bracketing

- A derivative-free method for *univariate* f
- works only on **unimodal** f
- (Draw choosing initial points and where to move next)

1.2 The Golden Ratio or Bracketing Search for 1D problems

- A derivative-free method
- a Bracketing method
  - find the local minimum of f on $[a, b]$
  - select 2 interior points c, d such that $a < c < d < b$
    * $f(c) \leq f(d) \implies$ min must lie in $[a, d]$. replace b with d, start again with $[a, d]$
    * $f(c) > f(d) \implies$ min must lie in $[c, b]$. replace a with c, start again with $[c, b]$
  - how to choose b, d though?
  - we want the length of the interval to be independent of whether we replace upper or lower bound
  - we want to reuse the non-replaced point from the previous iteration.
  - these imply the golden rule:
  - new point $x_i = a + \alpha_i(b - a)$, where $\alpha_1 = \frac{3-\sqrt{5}}{2}, \alpha_2 = \frac{\sqrt{5}-1}{2}$
  - α_2 is known as the *golden ratio*, well known for it's role in renaissance art.

```
In [1]: using Plots
        using Optim
        plotlyjs()
        f(x) = exp(x) - x^4
        minf(x) = -f(x)
        brent = optimize(minf,0,2,Brent())
        golden = optimize(minf,0,2,GoldenSection())
```

```
println("brent = $brent")
println("golden = $golden")
plot(f,0,2)
```

```
brent = Results of Optimization Algorithm
 * Algorithm: Brent's Method
 * Search Interval: [0.000000, 2.000000]
 * Minimizer: 8.310315e-01
 * Minimum: -1.818739e+00
 * Iterations: 12
 * Convergence: max(|x - x_upper|, |x - x_lower|) <= 2*(1.5e-08*|x|+2.2e-16): true
 * Objective Function Calls: 13
golden = Results of Optimization Algorithm
 * Algorithm: Golden Section Search
 * Search Interval: [0.000000, 2.000000]
 * Minimizer: 8.310315e-01
 * Minimum: -1.818739e+00
 * Iterations: 37
 * Convergence: max(|x - x_upper|, |x - x_lower|) <= 2*(1.5e-08*|x|+2.2e-16): true
 * Objective Function Calls: 38
```

1.2.1 Bisection Methods

- Root finding: `Roots.jl`
- Root finding in multivariate functions: `IntervalRootFinding.jl`

In [2]:
```
using Roots
#ăfind the zeros of this function:
f(x) = exp(x) - x^4
## bracketing
fzero(f, 8, 9)       # 8.613169456441398
fzero(f, -10, 0) # -0.8155534188089606
```

Out[2]: -0.8155534188089606

In [3]:
```
using IntervalRootFinding, IntervalArithmetic
-10..10
```

```
    ArgumentError: Module IntervalRootFinding not found in current path.
Run `Pkg.add("IntervalRootFinding")` to install the IntervalRootFinding package.



    Stacktrace:

     [1] _require(::Symbol) at ./loading.jl:435
```

```
 [2] require(::Symbol) at ./loading.jl:405

 [3] include_string(::String, ::String) at ./loading.jl:522
```

```
In [4]: X = IntervalBox(1..3, 2..4)
```

```
UndefVarError: IntervalBox not defined



Stacktrace:

 [1] include_string(::String, ::String) at ./loading.jl:522
```

```
In [5]: a = @interval(0.1, 0.3)
        b = @interval(0.3, 0.6)
        a + b
```

```
UndefVarError: @interval not defined



Stacktrace:

 [1] include_string(::String, ::String) at ./loading.jl:522
```

```
In [6]: rts = IntervalRootFinding.roots(x->x^2 - 2, -10..10, Bisection)
```

```
UndefVarError: IntervalRootFinding not defined



Stacktrace:

 [1] include_string(::String, ::String) at ./loading.jl:522
```

1.3 Rosenbrock Banana and Optim.jl

- We can supply the objective function and - depending on the solution algorithm - the gradient and hessian as well.

```
In [7]: using Optim
        using OptimTestProblems
        for (name, prob) in MultivariateProblems.UnconstrainedProblems.examples
           println(name)
        end
```

```
Rosenbrock
Quadratic Diagonal
Hosaki
Large Polynomial
Penalty Function I
Beale
Extended Rosenbrock
Polynomial
Powell
Exponential
Paraboloid Diagonal
Paraboloid Random Matrix
Extended Powell
Trigonometric
Fletcher-Powell
Parabola
Himmelblau
```

```
In [8]: rosenbrock = MultivariateProblems.UnconstrainedProblems.examples["Rosenbrock"]
```

```
Out[8]: OptimTestProblems.MultivariateProblems.OptimizationProblem{Void,Void,Float64,String,Void
```

1.4 Comparison Methods

- We will now look at a first class of algorithms, which are very simple, but sometimes a good starting point.
- They just *compare* function values.
- *Grid Search* : Compute the objective function at $G = \{x_1, \ldots, x_N\}$ and pick the highest value of f.
  - This is very slow.
  - It requires large N.
  - But it's robust (will find global optimizer for large enough N)

```
In [9]: # grid search on rosenbrock
        grid = collect(-1.0:0.1:3);
        grid2D = [[i;j] for i in grid,j in grid];
        val2D = map(rosenbrock.f,grid2D);
        r = findmin(val2D);
        println("grid search results in minimizer = $(grid2D[r[2]])")
```

```
grid search results in minimizer = [1.0, 1.0]
```

1.5 Local Descent Methods

- Applicable to multivariate problems
- We are searching for a *local model* that provides some guidance in a certain region of f over **where to go to next**.
- Gradient and Hessian are informative about this.

1.5.1 Local Descent Outline

All descent methods follow more or less this structure. At iteration k,

1. Check if candidate $\mathbf{x}^{(k)}$ satisfies stopping criterion:
    - if yes: stop
    - if no: continue
2. Get the local *descent direction* $\mathbf{d}^{(k)}$, using gradient, hessian, or both.
3. Set the *step size*, i.e. the length of the next step, α^k
4. Get the next candidate via

$$\mathbf{x}^{(k+1)} \longleftarrow \alpha^k \mathbf{d}^{(k)}$$

1.5.2 The Line Search Strategy

- An algorithm from the line search class chooses a direction $\mathbf{d}^{(k)} \in \mathbb{R}^n$ and searches along that direction starting from the current iterate $x_k \in \mathbb{R}^n$ for a new iterate $x_{k+1} \in \mathbb{R}^n$ with a lower function value.
- After deciding on a direction $\mathbf{d}^{(k)}$, one needs to decide the *step length* α to travel by solving

$$\min_{\alpha>0} f(x_k + \alpha \mathbf{d}^{(k)})$$

- In practice, solving this exactly is too costly, so algos usually generate a sequence of trial values α and pick the one with the lowest f.

In [10]:
```
# https://github.com/JuliaNLSolvers/LineSearches.jl
using LineSearches

algo_hz = Newton(linesearch = HagerZhang())
res_hz = Optim.optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!, rosenbrock.initial_
```

Out[10]:
```
Results of Optimization Algorithm
 * Algorithm: Newton's Method
 * Starting Point: [-1.2,1.0]
 * Minimizer: [1.0000000000000033,1.0000000000000067]
 * Minimum: 1.109336e-29
 * Iterations: 23
 * Convergence: true
   * |x - x'|  1.0e-32: false
     |x - x'| = 1.13e-08
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
     |f(x) - f(x')| = 6.35e+13 |f(x)|
```

```
    * |g(x)|  1.0e-08: true
      |g(x)| = 6.66e-15
    * Stopped by an increasing objective: false
    * Reached Maximum Number of Iterations: false
  * Objective Calls: 71
  * Gradient Calls: 71
  * Hessian Calls: 23
```

1.5.3 The Trust Region Strategy

- First choose max step size, then the direction
- Finds the next step $\mathbf{x}^{(k+1)}$ by minimizing a model of $\hat{f}$ over a *trust region*, centered on $\mathbf{x}^{(k)}$
  - 2nd order Tayloer approx of f is common.
- Radius δ of trust region is changed based on how well $\hat{f}$ fits f in trust region.
- Get $\mathbf{x}'$ via

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

In [11]:
```
# Optim.jl has a TrustRegion for Newton (see below for Newton's Method)
NewtonTrustRegion(; initial_delta = 1.0, # The starting trust region radius
                    delta_hat = 100.0, # The largest allowable trust region radius
                    eta = 0.1, #When rho is at least eta, accept the step.
                    rho_lower = 0.25, # When rho is less than rho_lower, shrink the tru
                    rho_upper = 0.75) # When rho is greater than rho_upper, grow the tr
res = Optim.optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!, rosenbrock.initial_x,
```

Out[11]:
```
Results of Optimization Algorithm
 * Algorithm: Newton's Method (Trust Region)
 * Starting Point: [-1.2,1.0]
 * Minimizer: [0.9999999994405535,0.9999999988644926]
 * Minimum: 3.405841e-19
 * Iterations: 25
 * Convergence: true
   * |x - x'|  1.0e-32: false
     |x - x'| = 8.84e-06
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
     |f(x) - f(x')| = 1.87e+08 |f(x)|
   * |g(x)|  1.0e-08: true
     |g(x)| = 5.53e-09
   * Stopped by an increasing objective: false
   * Reached Maximum Number of Iterations: false
 * Objective Calls: 26
 * Gradient Calls: 26
 * Hessian Calls: 22
```

1.5.4 Stopping criteria

1. maximum number of iterations reached

2. absolute improvement $|f(x) - f(x')| \leq \epsilon$
3. relative improvement $|f(x) - f(x')|/|f(x)| \leq \epsilon$
4. Gradient close to zero $|g(x)| \approx 0$

1.5.5 Gradient Descent

- Here we define
$$\mathbf{g}^{(k)} = \nabla f(\mathbf{d}^{(k)})$$
- And our descent becomes
$$\mathbf{d}^{(k)} = -\nabla \frac{\mathbf{g}^{(k)}}{\|\mathbf{g}^{(k)}\|}$$
- Minimizing wrt step size results in a jagged path (each direction is orthogonal to previous direction!)
$$\alpha^{(k)} = \arg\min \alpha f(\mathbf{x}^{(k)} + \alpha \mathbf{d}^{(k)})$$
- *Conjugate* Gradient avoids this issue.

In [12]:
```
# Optim.jl again
GradientDescent(; alphaguess = LineSearches.InitialPrevious(),
                  linesearch = LineSearches.HagerZhang(),
                  P = nothing,
                  precondprep = (P, x) -> nothing)
```

Out[12]:
```
Optim.GradientDescent{LineSearches.InitialPrevious{Float64},LineSearches.HagerZhang{Flo
  alpha: Float64 1.0
  alphamin: Float64 0.0
  alphamax: Float64 Inf
, LineSearches.HagerZhang{Float64}
  delta: Float64 0.1
  sigma: Float64 0.9
  alphamax: Float64 Inf
  rho: Float64 5.0
  epsilon: Float64 1.0e-6
  gamma: Float64 0.66
  linesearchmax: Int64 50
  psi3: Float64 0.1
  display: Int64 0
, nothing, #5, Optim.Flat())
```

In [13]:
```
# there is a dedicated LineSearch package: https://github.com/JuliaNLSolvers/LineSearch
GD = optimize(rosenbrock.f, rosenbrock.g!,[0.0, 0.0],GradientDescent())
GD1 = optimize(rosenbrock.f, rosenbrock.g!,[0.0, 0.0],GradientDescent(),Optim.Options(i
GD2 = optimize(rosenbrock.f, rosenbrock.g!,[0.0, 0.0],GradientDescent(),Optim.Options(i

println("gradient descent = $GD")
println("\n")
println("gradient descent 2 = $GD1")
println("\n")
println("gradient descent 3 = $GD2")
```

```
gradient descent = Results of Optimization Algorithm
 * Algorithm: Gradient Descent
 * Starting Point: [0.0,0.0]
 * Minimizer: [0.9356732500354086,0.875073922357589]
 * Minimum: 4.154782e-03
 * Iterations: 1000
 * Convergence: false
   * |x - x'|  1.0e-32: false
     |x - x'| = 1.82e-04
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
     |f(x) - f(x')| = 1.97e-03 |f(x)|
   * |g(x)|  1.0e-08: false
     |g(x)| = 8.21e-02
   * Stopped by an increasing objective: false
   * Reached Maximum Number of Iterations: true
 * Objective Calls: 2532
 * Gradient Calls: 2532


gradient descent 2 = Results of Optimization Algorithm
 * Algorithm: Gradient Descent
 * Starting Point: [0.0,0.0]
 * Minimizer: [0.9978398797724763,0.9956717950747302]
 * Minimum: 4.682073e-06
 * Iterations: 5000
 * Convergence: false
   * |x - x'|  1.0e-32: false
     |x - x'| = 5.08e-06
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
     |f(x) - f(x')| = 1.62e-03 |f(x)|
   * |g(x)|  1.0e-08: false
     |g(x)| = 2.53e-03
   * Stopped by an increasing objective: false
   * Reached Maximum Number of Iterations: true
 * Objective Calls: 12532
 * Gradient Calls: 12532


gradient descent 3 = Results of Optimization Algorithm
 * Algorithm: Gradient Descent
 * Starting Point: [0.0,0.0]
 * Minimizer: [0.9999999914304203,0.9999999828109042]
 * Minimum: 7.368706e-17
 * Iterations: 20458
 * Convergence: true
   * |x - x'|  1.0e-32: false
     |x - x'| = 2.00e-11
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
```

```
    |f(x) - f(x')| = 1.61e-03 |f(x)|
  * |g(x)|  1.0e-08: true
    |g(x)| = 9.99e-09
  * Stopped by an increasing objective: false
  * Reached Maximum Number of Iterations: false
 * Objective Calls: 51177
 * Gradient Calls: 51177
```

1.6 Second Order Methods

1.6.1 Newton's Method

- We start with a 2nd order Taylor approx over x at step k:

$$q(x) = f(x^{(k)}) + (x - x^{(k)})f'(x^{(k)}) + \frac{(x - x^{(k)})^2}{2} f''(x^{(k)})$$

- We set find it's root and rearrange to find the next step $k+1$:

$$\frac{\partial q(x)}{\partial x} = f'(x^{(k)}) + (x - x^{(k)})f''(x^{(k)}) = 0$$
$$x^{(k+1)} = x^{(k)} - \frac{f'(x^{(k)})}{f''(x^{(k)})}$$

- The same argument works for multidimensional functions by using Hessian and Gradient
- We would get a descent $\mathbf{d}^k$ by setting:

$$\mathbf{d}^k = -\frac{\mathbf{g}^k}{\mathbf{H}^k}$$

- There are several options to avoid (often costly) computation of the Hessian $\mathbf{H}$:

1. Quasi-Newton updates $\mathbf{H}$ starting from identity matrix
2. Broyden-Fletcher-Goldfarb-Shanno (BFGS) does better with approx linesearch
3. L-BFGS is the limited memory version for large problems

```
In [14]: optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!, [0.0, 0.0], Newton(),Optim.Options
```

```
Iter     Function value   Gradient norm
     0     1.000000e+00     2.000000e+00
     1     8.431140e-01     1.588830e+00
     2     6.776980e-01     3.453340e+00
     3     4.954645e-01     4.862093e+00
     4     3.041921e-01     2.590086e+00
     5     1.991512e-01     3.780900e+00
     6     9.531907e-02     1.299090e+00
     7     5.657827e-02     2.445401e+00
     8     2.257807e-02     1.839332e+00
     9     6.626125e-03     1.314236e+00
    10     8.689753e-04     5.438279e-01
```

```
    11     4.951399e-06     7.814556e-02
    12     9.065070e-10     6.017046e-04
    13     9.337686e-18     1.059738e-07
    14     3.081488e-31     1.110223e-15
```

```
Out[14]: Results of Optimization Algorithm
          * Algorithm: Newton's Method
          * Starting Point: [0.0,0.0]
          * Minimizer: [0.9999999999999994,0.9999999999999989]
          * Minimum: 3.081488e-31
          * Iterations: 14
          * Convergence: true
            * |x - x'|  1.0e-32: false
              |x - x'| = 3.06e-09
            * |f(x) - f(x')|  1.0e-32 |f(x)|: false
              |f(x) - f(x')| = 3.03e+13 |f(x)|
            * |g(x)|  1.0e-08: true
              |g(x)| = 1.11e-15
            * Stopped by an increasing objective: false
            * Reached Maximum Number of Iterations: false
          * Objective Calls: 44
          * Gradient Calls: 44
          * Hessian Calls: 14
```

```
In [15]: @show optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!,  [-1.0, 3.0], BFGS());
```

```
optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!, [-1.0, 3.0], BFGS()) = Results of Optimizat
 * Algorithm: BFGS
 * Starting Point: [-1.0,3.0]
 * Minimizer: [0.9999999999999956,0.999999999999987]
 * Minimum: 1.707144e-27
 * Iterations: 39
 * Convergence: true
   * |x - x'|  1.0e-32: false
     |x - x'| = 1.54e-08
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
     |f(x) - f(x')| = 3.55e+10 |f(x)|
   * |g(x)|  1.0e-08: true
     |g(x)| = 1.63e-12
   * Stopped by an increasing objective: false
   * Reached Maximum Number of Iterations: false
 * Objective Calls: 137
 * Gradient Calls: 137
```

```
In [16]: # low memory BFGS
         @show optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!,  [0.0, 0.0], LBFGS());
```

```
optimize(rosenbrock.f, rosenbrock.g!, rosenbrock.h!, [0.0, 0.0], LBFGS()) = Results of Optimizat
 * Algorithm: L-BFGS
 * Starting Point: [0.0,0.0]
 * Minimizer: [0.999999999999928,0.9999999999998559]
 * Minimum: 5.191703e-27
 * Iterations: 24
 * Convergence: true
   * |x - x'|  1.0e-32: false
     |x - x'| = 4.58e-11
   * |f(x) - f(x')|  1.0e-32 |f(x)|: false
     |f(x) - f(x')| = 8.50e+07 |f(x)|
   * |g(x)|  1.0e-08: true
     |g(x)| = 1.44e-13
   * Stopped by an increasing objective: false
   * Reached Maximum Number of Iterations: false
 * Objective Calls: 67
 * Gradient Calls: 67
```

1.7 Direct Methods

- No derivative information is used - *derivative free*
- If it's very hard / impossible to provide gradient information, this is our only chance.
- Direct methods use other criteria than the gradient to inform the next step (and ulimtately convergence).

1.7.1 Cyclic Coordinate Descent -- Taxicab search

- We do a line search over each dimension, one after the other
- *taxicab* because the path looks like a NYC taxi changing direction at each block.
- given $\mathbf{x}^{(1)}$, we proceed

$$\mathbf{x}^{(2)} = \arg\min_{x_1} f(x_1, x_2^{(1)}, \ldots, x_n^{(1)})$$
$$\mathbf{x}^{(3)} = \arg\min_{x_2} f(x_1^{(2)}, x_2, x_3^{(2)} \ldots, x_n^{(2)})$$

- unfortunately this can easily get stuck because it can only move in 2 directions.

```
In [17]: # start to setup a basis function, i.e. unit vectors to index each direction:
         basis(i, n) = [k == i ? 1.0 : 0.0 for k in 1 : n]
         function cyclic_coordinate_descent(f, x, )
             , n = Inf, length(x)
             while abs() > 
                 x = copy(x)
                     for i in 1 : n
                         d = basis(i, n)
                         x = line_search(f, x, d)
                     end
                   = norm(x - x)
```

```
        end
        return x
    end
```

Out[17]: cyclic_coordinate_descent (generic function with 1 method)

1.7.2 General Pattern Search

- We search according to an arbitrary *pattern* $\mathcal{P}$ of candidate points, anchored at current guess $\mathbf{x}$.
- With step size α and set $\mathcal{D}$ of directions

$$\mathcal{P} = \mathbf{x} + \alpha\mathbf{d} \text{ for } \mathbf{d} \in \mathcal{D}$$

- Convergence is guaranteed under conditions:
  - $\mathcal{D}$ must be a positive spanning set: at least one $\mathbf{d} \in \mathcal{D}$ has a non-zero gradient.

In [18]:
```
function generalized_pattern_search(f, x, , D, , =0.5)
    y, n = f(x), length(x)
    evals = 0
    while  > 
        improved = false
        for (i,d) in enumerate(D)
            x = x + *d
            y = f(x)
            evals += 1
            if y < y
                x, y, improved = x, y, true
                D = unshift!(deleteat!(D, i), d)
                break
            end
        end
        if !improved
             *= 
        end
    end
    println("$evals evaluations")
    return x
end
```

Out[18]: generalized_pattern_search (generic function with 2 methods)

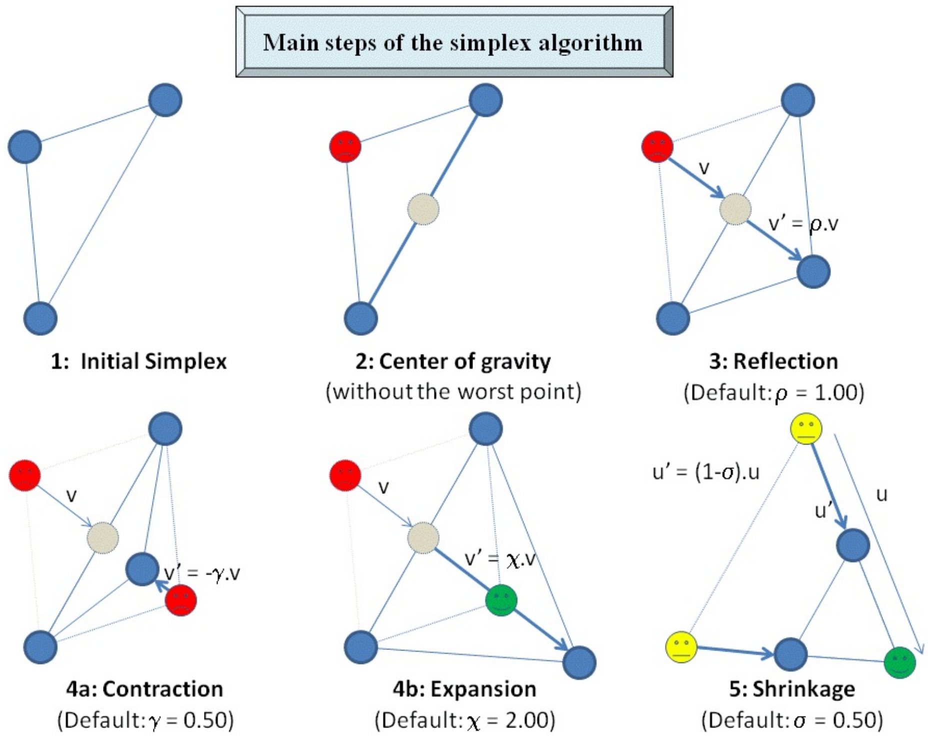
In [19]:
```
D = [[1,0],[0,1],[-1,-0.5]]
D = [[1,0],[0,1]]
y=generalized_pattern_search(rosenbrock.f,zeros(2),0.8,D,1e-6 )
```

```
11923 evaluations
```

Out[19]:
```
2-element Array{Float64,1}:
 0.999673
 0.999347
```

1.8 Bracketing for Multidimensional Problems: Nelder-Mead

- The Goal here is to find the simplex containing the local minimizer x^*
- In the case where f is n-D, this simplex has $n + 1$ vertices
- In the case where f is 2-D, this simplex has $2 + 1$ vertices, i.e. it's a triangle.
- The method proceeds by evaluating the function at all $n + 1$ vertices, and by replacing the worst function value with a new guess.
- this can be achieved by a sequence of moves:
  - reflect
  - expand
  - contract
  - shrink movements.



- this is a very popular method. The matlab functions `fmincon` and `fminsearch` implements it.
- When it works, it works quite fast.
- No derivatives required.

```
In [20]: nm=optimize(rosenbrock.f, [0.0, 0.0], NelderMead());
         nm.minimizer
```

```
Out[20]: 2-element Array{Float64,1}:
          0.999963
          0.999932
```

- But.

1.9 Bracketing for Multidimensional Problems: Comment on Nelder-Mead

Lagarias et al. (SIOPT, 1999): At present there is no function in any dimension greater than one, for which the original Nelder-Mead algorithm has been proved to converge to a minimizer.

Given all the known inefficiencies and failures of the Nelder-Mead algorithm [...], one might wonder why it is used at all, let alone why it is so extraordinarily popular.

1.10 things to read up on

- Divided Rectangles (DIRECT)
- simulated annealing and other stochastic gradient methods

1.11 Stochastic Optimization Methods

- Gradient based methods like steepest descent may be susceptible to getting stuck at local minima.
- Randomly shocking the value of the descent direction may be a solution to this.
- For example, one could modify our gradient descent from before to become

$$\mathbf{x}^{(k+1)} \longleftarrow \mathbf{x}^{(k)} + \alpha^k \mathbf{g}^{(k)} + ''^{(k)}$$

- where $''^{(k)} \sim N(0, \sigma_k^2)$, decreasing with k.
- This *stochastic gradient descent* is often used when training neural networks.

1.11.1 Simulated Annealing

- We specify a *temperature* that controls the degree of randomness.
- At first the temperature is high, letting the search jump around widely. This is to escape local minima.
- The temperature is gradually decreased, reducing the step sizes. This is to find the local optimimum in the *best* region.
- At every iteration k, we accept new point $\mathbf{x}'$ with

$$\Pr(\text{accept } \mathbf{x}') = \begin{cases} 1 & \text{if } \Delta y \leq 0 \\ \min(e^{\Delta y/t}, 1) & \text{if } \Delta y > 0 \end{cases}$$

- here $\Delta y = f(\mathbf{x}') - f(\mathbf{x})$, and t is the *temperature*.
- $\Pr(\text{accept } \mathbf{x}')$ is called the **Metropolis Criterion**, building block of *Accept/Reject* algorithms.

In [21]:
```
#ăf: function
# x: initial point
# T: transition distribution
#ăt: temp schedule, k_max: max iterations
function simulated_annealing(f, x, T, t, k_max)
    y = f(x)
    ytrace = zeros(typeof(y),k_max)
```

```
        x_best, y_best = x, y
        for k in 1 : k_max
            x = x + rand(T)
            y = f(x)
            y = y - y
            if y  0 || rand() < exp(-y/t(k))
                x, y = x, y
            end
            if y < y_best
                x_best, y_best = x, y
            end
            ytrace[k] = y_best
        end
        return x_best,ytrace
    end
```

Out[21]: simulated_annealing (generic function with 1 method)

In [22]:
```
function ackley(x, a=20, b=0.2, c=2)
    d = length(x)
    return -a*exp(-b*sqrt(sum(x.^2)/d)) - exp(sum(cos.(c*xi) for xi in x)/d) + a + e
end
using Plots
plotlyjs()
surface(-30:0.1:30,-30:0.1:30,(x,y)->ackley([x, y]))
```

In [23]:
```
using Distributions
d = Dict()
for sig in (1,5,25), t1 in (1,10,25)
    tmp = [simulated_annealing(ackley,[15,15],MvNormal(2,sig),x->t1/x,100) for i in 1:3
    d[(sig,t1)] = Dict()
    d[(sig,t1)][:y] = mapslices(x->ackley(x),hcat([tmp[i][1] for i in 1:300]...),[1])
    d[(sig,t1)][:ytrace] = hcat([tmp[i][2] for i in 1:300]...)
end
d

# x=[simulated_annealing(ackley,[15,15],MvNormal(2,1),x->1.0/x,100) for i in 1:100]
# y=[simulated_annealing(ackley,[15,15],MvNormal(2,5),x->10.0/x,100) for i in 1:100]
# map((x)->ackley([x[1],x[2] ]),y)
```

Out[23]:
```
Dict{Any,Any} with 9 entries:
  (5, 25)  => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (5, 10)  => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (1, 25)  => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (5, 1)   => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (25, 1)  => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (25, 25) => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (1, 1)   => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (1, 10)  => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
  (25, 10) => Dict{Any,Any}(Pair{Any,Any}(:ytrace, [19.0043 19.0043  19.0043 1
```

2 Constraints

Recall our core optimization problem:

$$\min_{x \in \mathbb{R}^n} f(x) \text{ s.t. } x \in \mathcal{X}$$

- Up to now, the feasible set was $\mathcal{X} \in \mathbb{R}^n$.
- In **constrained problems** $\mathcal{X}$ is a subset thereof.
- We already encountered *box constraints*, e.g. $x \in [a, b]$.
- Sometimes the contrained solution coincides with the unconstrained one, sometimes it does not.
- There are *equality constraints* and *inequality constraints*.

2.1 Lagrange Multipliers

- Used to optimize a function subject to equality constraints.

$$\min_x f(x)$$
$$\text{subject to } h(x) = 0$$

where both f and h have continuous partial derivatives.

- We look for contour lines of f that are aligned to contours of $h(x) = 0$.

In other words, we want to find the best x s.t. $h(x) = 0$ and we have

$$\nabla f(x) = \lambda \nabla h(x)$$

for some *Lagrange Mutliplier* λ * Notice that we need the scalar λ because the magnitudes of the gradients may be different. * We therefore form the the **Lagrangian**:

$$\mathcal{L}(x, \lambda) = f(x) - \lambda h(x)$$

2.1.1 Example

Suppose we have

$$\min_x - \exp\left(-\left(x_1 x_2 - \frac{3}{2}\right)^2 - \left(x_2 - \frac{3}{2}\right)^2\right)$$
$$\text{subject to } x_1 - x_2^2 = 0$$

We form the Lagrangiagn:

$$\mathcal{L}(x_1, x_2, \lambda) = -\exp\left(-\left(x_1 x_2 - \frac{3}{2}\right)^2 - \left(x_2 - \frac{3}{2}\right)^2\right) - \lambda(x_1 - x_2^2)$$

Then we compute the gradient wrt to x_1, x_2, λ, set to zero and solve.

```
In [35]: gr()
         f(x1,x2) = -exp.(-(x1.*x2 - 3/2).^2 - (x2-3/2).^2)
         c(x1) = sqrt(x1)
         x=0:0.01:3.5
         contour(x,x,(x,y)->f(x,y),lw=1.5,levels=[collect(0:-0.1:-0.85)...,-0.887,-0.95,-1])
         plot!(c,0.01,3.5,label="",lw=2,color=:black)
         scatter!([1.358],[1.165],markersize=5,markercolor=:red,label="Constr. Optimum")
```

- If we had multiple constraints (l), we'd just add them up to get

$$\mathcal{L}(\mathbf{x},\breve{\ }) = f(\mathbf{x}) - \sum_{i=1}^{l} \lambda_i h_i(\mathbf{x})$$

2.2 Inequality Constraints

Suppose now we had

$$\min_{\mathbf{x}} f(\mathbf{x})$$
$$\text{subject to } g(\mathbf{x}) \leq 0$$

which, if the solution lies right on the constraint *boundary*, means that

$$\nabla f - \mu \nabla g = 0$$

for some scalar μ - as before.

- In this case, we say the **constraint is active**.
- In the opposite case, i.e. the solution lies **inside** the contrained region, we way the contraint is **inactive**.
- In that case, we are back to an *unconstrained* problem, look for $\nabla f = 0$, and set $\mu = 0$.

```
In [38]: #ăthe blue area shows the FEASIBLE SET
         contour(x,x,(x,y)->f(x,y),lw=1.5,levels=[collect(0:-0.1:-0.85)...,-0.887,-0.95,-1])
         plot!(c,0.01,3.5,label="",lw=2,color=:black,fill=(0,0.5,:blue))
         scatter!([1.358],[1.165],markersize=5,markercolor=:red,label="Constr. Optimum")
```

```
In [39]: #ăthe blue area shows the FEASIBLE SET
         #ăNOW THE CONSTRAINT IS INACTIVE OR SLACK!
         c2(x1) = 1+sqrt(x1)
         contour(x,x,(x,y)->f(x,y),lw=1.5,levels=[collect(0:-0.1:-0.85)...,-0.887,-0.95,-1])
         plot!(c2,0.01,3.5,label="",lw=2,color=:black,fill=(0,0.5,:blue))
         scatter!([1],[1.5],markersize=5,markercolor=:red,label="Unconstr. Optimum")
```

2.3 Infinity Step

- We could do an **infinite step** to avoid *infeasible points*:

$$
\begin{aligned}
f_{\infty\text{-step}} &= \begin{cases} f(\mathbf{x}) & \text{if } g(\mathbf{x}) \leq 0 \\ \infty & \text{else.} \end{cases} \\
&= f(\mathbf{x}) + \infty(g(\mathbf{x} > 0)
\end{aligned}
$$

- Unfortunately, this is discontinous and non-differentiable, i.e. hard to handle for algorithms.
- Instead, we use a *linear penalty* $\mu g(\mathbf{x})$ on the objective if the constraint is violated.
- The penalty provides a lower bound to ∞:

$$
\mathcal{L}(\mathbf{x}, \mu) = f(\mathbf{x}) + \mu g(\mathbf{x})
$$

- We can get back the infinite step by maximizing the penalty:

$$
f_{\infty\text{-step}} = \max_{\mu \geq 0} \mathcal{L}(\mathbf{x}, \mu)
$$

- Every infeasible $\mathbf{x}$ returns ∞, all others return $f(\mathbf{x})$

2.4 Kuhn-Karush-Tucker (KKT)

- Our problem thus becomes

$$
\min_{\mathbf{x}} \max_{\mu \geq 0} \mathcal{L}(\mathbf{x}, \mu)
$$

- This is called the **primal problem**. Optimizing this requires:

1. $g(\mathbf{x}^*) \leq 0$. Point is feasible.
2. $\mu \geq 0$. Penalty goes into the right direction. *Dual feasibility*.
3. $\mu g(\mathbf{x}^*) = 0$. Feasible point on the boundary has $g(\mathbf{x}) = 0$, otherwise $g(\mathbf{x}) < 0$ and $\mu = 0$.
4. $\nabla f(\mathbf{x}^*) - \mu \nabla g(\mathbf{x}^*) = 0$. With an active constraint, we want parallel contours of objective and constraint. When inactive, our optimum just has $\nabla f(\mathbf{x}^*) = 0$, which means $\mu = 0$.

The preceding four conditions are called the Kuhn-Karush-Tucker (KKT) conditions. In the above order, and in general terms, they are:

1. Feasibility
2. Dual Feasibility
3. Complementary Slackness
4. Stationarity.

The KKT conditions are the FONCs for problems with smooth constraints.

2.5 Duality

We can combine equality and inequality constraints:

$$\mathcal{L}(\mathbf{x}, \breve{}, \bar{}) = f(\mathbf{x}) + \sum_i \lambda_i h_i(\mathbf{x}) + \sum_j \mu_j g_j(\mathbf{x})$$

where, notice, we reverted the sign of λ since this is unrestricted.

- The Primal problem is identical to the original problem and just as difficult to solve:

$$\min_{\mathbf{x}} \max_{\bar{} \geq 0, \breve{}} \mathcal{L}(\mathbf{x}, \bar{}, \breve{})$$

- The Dual problem reverses min and max:

$$\max_{\bar{} \geq 0, \breve{}} \min_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \bar{}, \breve{})$$

2.5.1 Dual Values

- The *max-min-inequality* states that for any function $f(a, b)$

$$\max_{\mathbf{a}} \min_{\mathbf{b}} f(\mathbf{a}, \mathbf{b}) \leq \min_{\mathbf{b}} \max_{\mathbf{a}} f(\mathbf{a}, \mathbf{b})$$

- Hence, the solution to the dual is a lower bound to the solution of the primal problem.
- The solution to the *dual function*, $\min_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \bar{}, \breve{})$ is the min of a collection of linear functions, and thus always concave.
- It is easy to optimize this.
- In general, solving the dual is easy whenever minimizing $\mathcal{L}$ wrt x is easy.

2.6 Penalty Methods

- We can convert the constrained problem back to unconstrained by adding penalty terms for constraint violoations.
- A simple method could just count the number of violations:

$$p_{\text{count}}(\mathbf{x}) = \sum_i (h_i(\mathbf{x}) \neq 0) + \sum_j (g_j(\mathbf{x} > 0)$$

- and add this to the objective in an *unconstrained* problem with penalty $\rho > 0$

$$\min_{\mathbf{x}} f(\mathbf{x}) + \rho p_{\text{count}}(\mathbf{x})$$

- One can choose the penalty function: for example, a quadratic penaly will produce a smooth objective function
- Notice that ρ needs to become very large sometimes here.

2.7 Augmented Lagrange Method

- This is very similar, but specific to equality constraints.

2.8 Interior Point Method

- Also called *barrier method*.
- These methods make sure that the search point remains always feasible.
- As one approaches the constraint boundary, the barrier function goes to infinity. Properties:

1. $p_{\text{barrier}}(\mathbf{x})$ is continuous
2. $p_{\text{barrier}}(\mathbf{x})$ is non negative
3. $p_{\text{barrier}}(\mathbf{x})$ goes to infinitey as one approaches the constraint boundary

2.8.1 Barriers

- Inverse Barrier

$$p_{\text{barrier}}(\mathbf{x}) = -\sum_i \frac{1}{g_i(\mathbf{x})}$$

- Log Barrier

$$p_{\text{barrier}}(\mathbf{x}) = -\sum_i \begin{cases} \log(-g_i(\mathbf{x})) & \text{if } g_i(\mathbf{x}) \geq -1 \\ 0 & \text{else.} \end{cases}$$

- The approach is as before, one transforms the problem to an unconstrained one and increases ρ until convergence:

$$\min_{\mathbf{x}} f(\mathbf{x}) + \frac{1}{\rho} p_{\text{barrier}}(\mathbf{x})$$

2.8.2 Examples

$$\min_{x \in \mathbb{R}^2} \sqrt{x_2} \text{ subject to } \begin{array}{r} x_2 \geq 0 \\ x_2 \geq (a_1 x_1 + b_1)^3 \\ x_2 \geq (a_2 x_1 + b_2)^3 \end{array}$$

2.9 Constrained Optimisation with `NLopt.jl`

- We need to specify one function for each objective and constraint.
- Both of those functions need to compute the function value (i.e. objective or constraint) *and* it's respective gradient.
- `NLopt` expects contraints **always** to be formulated in the format

$$g(x) \leq 0$$

where g is your constraint function

- The constraint function is formulated for each constraint at x. it returns a number (the value of the constraint at x), and it fills out the gradient vector, which is the partial derivative of the current constraint wrt x.
- There is also the option to have vector valued constraints, see the documentation.
- We set this up as follows:

In [27]:
```
using NLopt

count = 0 # keep track of # function evaluations

function myfunc(x::Vector, grad::Vector)
    if length(grad) > 0
        grad[1] = 0
        grad[2] = 0.5/sqrt(x[2])
    end

    global count
    count::Int += 1
    println("f_$count($x)")

    sqrt(x[2])
end

function myconstraint(x::Vector, grad::Vector, a, b)
    if length(grad) > 0
        grad[1] = 3a * (a*x[1] + b)^2
        grad[2] = -1
    end
    (a*x[1] + b)^3 - x[2]
end

opt = Opt(:LD_MMA, 2)
lower_bounds!(opt, [-Inf, 0.])
xtol_rel!(opt,1e-4)

min_objective!(opt, myfunc)
inequality_constraint!(opt, (x,g) -> myconstraint(x,g,2,0), 1e-8)
inequality_constraint!(opt, (x,g) -> myconstraint(x,g,-1,1), 1e-8)

(minfunc,minx,ret) = NLopt.optimize(opt, [1.234, 5.678])
println("got $minfunc at $minx after $count iterations (returned $ret)")
```

```
f_1([1.234, 5.678])
f_2([0.878739, 5.55137])
f_3([0.826216, 5.0439])
f_4([0.473944, 4.07677])
f_5([0.353898, 3.03085])
f_6([0.333873, 1.97179])
```

```
f_7([0.333334, 1.04509])
f_8([0.333334, 0.469503])
f_9([0.333333, 0.305792])
f_10([0.333333, 0.296322])
f_11([0.333333, 0.296296])
got 0.5443310477213124 at [0.333333, 0.296296] after 11 iterations (returned XTOL_REACHED)


WARNING: using NLopt.optimize in module Main conflicts with an existing identifier.
```

2.10 NLopt: Rosenbrock

- Let's tackle the rosenbrock example again.
- To make it more interesting, let's add an inequality constraint.

$$\min_{x \in \mathbb{R}^2} (1 - x_1)^2 + 100(x_2 - x_1^2)^2 \text{ subject to } 0.8 - x_1^2 - x_2^2 \geq 0$$

- in `NLopt` format, the constraint is $x_1 + x_2 - 0.8 \leq 0$

```
In [28]: function rosenbrockf(x::Vector,grad::Vector)
             if length(grad) > 0
                     grad[1] = -2.0 * (1.0 - x[1]) - 400.0 * (x[2] - x[1]^2) * x[1]
                     grad[2] = 200.0 * (x[2] - x[1]^2)
             end
             return (1.0 - x[1])^2 + 100.0 * (x[2] - x[1]^2)^2
         end
         function r_constraint(x::Vector, grad::Vector)
             if length(grad) > 0
                 grad[1] = 2*x[1]
                 grad[2] = 2*x[2]
                 end
                 return x[1]^2 + x[2]^2 - 0.8
         end
         opt = Opt(:LD_MMA, 2)
         lower_bounds!(opt, [-5, -5.0])
         min_objective!(opt,(x,g) -> rosenbrockf(x,g))
         inequality_constraint!(opt, (x,g) -> r_constraint(x,g))
         ftol_rel!(opt,1e-9)
         NLopt.optimize(opt, [-1.0,0.0])

Out[28]: (0.07588358473630112, [0.724702, 0.524221], :FTOL_REACHED)
```

2.11 JuMP.jl

- Introduce `JuMP.jl`
- JuMP is a mathematical programming interface for Julia. It is like AMPL, but for free and with a decent programming language.
- The main highlights are:

- It uses automatic differentiation to compute derivatives from your expression.
- It supplies this information, as well as the sparsity structure of the Hessian to your preferred solver.
- It decouples your problem completely from the type of solver you are using. This is great, since you don't have to worry about different solvers having different interfaces.
- In order to achieve this, `JuMP` uses `MathProgBase.jl`, which converts your problem formulation into a standard representation of an optimization problem.

- Let's look at the readme
- The technical citation is Lubin et al [**?**]

2.12 JuMP: Quick start guide

- this is form the quick start guide
- please check the docs, they are excellent.

2.12.1 Step 1: create a model

- A model collects variables, objective function and constraints.
- it defines a solver to be used.

```
using Clp
m = Model(solver=ClpSolver())  # provide a solver

#ăDefine variables
@variable(m, x )              # No bounds
@variable(m, x >= lb )        # Lower bound only (note: 'lb <= x' is not valid)
@variable(m, x <= ub )        # Upper bound only
@variable(m, lb <= x <= ub )  # Lower and upper bounds


# we can create arrays of a variable
N = 2
@variable(m, x[1:M,1:N] >= 0 )

# or put them in a block
@variables m begin
    x
    y >= 0
    Z[1:10], Bin
    X[1:3,1:3], SDP
    q[i=1:2], (lowerbound = i, start = 2i, upperbound = 3i)
    t[j=1:3], (Int, start = j)
end

# Equivalent to:
@variable(m, x)
@variable(m, y >= 0)
@variable(m, Z[1:10], Bin)
```

```
@variable(m, X[1:3,1:3], SDP)
@variable(m, q[i=1:2], lowerbound = i, start = 2i, upperbound = 3i)
@variable(m, t[j=1:3], Int, start = j)

# bounds can depend on indices
@variable(m, x[i=1:10] >= i )
```

2.13 Objective and Constraints

- We can easily add objective and constraint functions:

```
@constraint(m, x[i] - s[i] <= 0)  # Other options: == and >=
@constraint(m, sum(x[i] for i=1:numLocation) == 1)
@objective(m, Max, 5x + 22y + (x+y)/2) # or Min
```

- This is fully integrated with Julia. you can use the `generator` syntax for sums:

```
@objective(sum(x[i] + y[i]/pi for i = I1, j = I2 if i+j < some_val))
```

```
In [29]: ##ăSimple example
         using JuMP
         using Clp

         let
             m = Model(solver = ClpSolver())
             @variable(m, 0 <= x <= 2 )
             @variable(m, 0 <= y <= 30 )

             @objective(m, Max, 5x + 3*y )
             @constraint(m, 1x + 5y <= 3.0 )

             print(m)

             status = solve(m)

             println("Objective value: ", getobjectivevalue(m))
             println("x = ", getvalue(x))
             println("y = ", getvalue(y))
         end
```

```
Max 5 x + 3 y
Subject to
 x + 5 y  3
 0  x  2
 0  y  30
Objective value: 10.6
x = 2.0
y = 0.2
```

```
In [30]: # JuMP: Rosenbrock Example
         # Instead of hand-coding first and second derivatives, you only have to give `JuMP` exp
         # Here is an example.

         using Ipopt

         let

             m = Model(solver=IpoptSolver())

             @variable(m, x)
             @variable(m, y)

             @NLobjective(m, Min, (1-x)^2 + 100(y-x^2)^2)

             solve(m)

             println("x = ", getvalue(x), " y = ", getvalue(y))

         end
```

```
******************************************************************************
This program contains Ipopt, a library for large-scale nonlinear optimization.
 Ipopt is released as open source code under the Eclipse Public License (EPL).
         For more information visit http://projects.coin-or.org/Ipopt
******************************************************************************

This is Ipopt version 3.12.8, running with linear solver mumps.
NOTE: Other linear solvers might be more efficient (see Ipopt documentation).

Number of nonzeros in equality constraint Jacobian...:        0
Number of nonzeros in inequality constraint Jacobian.:        0
Number of nonzeros in Lagrangian Hessian...:        3

Total number of variables...:        2
                     variables with only lower bounds:        0
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints...:        0
Total number of inequality constraints...:        0
        inequality constraints with only lower bounds:        0
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0  1.0000000e+00 0.00e+00 2.00e+00  -1.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1  9.5312500e-01 0.00e+00 1.25e+01  -1.0 1.00e+00    -  1.00e+00 2.50e-01f  3
```

```
   2  4.8320569e-01 0.00e+00 1.01e+00  -1.0 9.03e-02    -  1.00e+00 1.00e+00f  1
   3  4.5708829e-01 0.00e+00 9.53e+00  -1.0 4.29e-01    -  1.00e+00 5.00e-01f  2
   4  1.8894205e-01 0.00e+00 4.15e-01  -1.0 9.51e-02    -  1.00e+00 1.00e+00f  1
   5  1.3918726e-01 0.00e+00 6.51e+00  -1.7 3.49e-01    -  1.00e+00 5.00e-01f  2
   6  5.4940990e-02 0.00e+00 4.51e-01  -1.7 9.29e-02    -  1.00e+00 1.00e+00f  1
   7  2.9144630e-02 0.00e+00 2.27e+00  -1.7 2.49e-01    -  1.00e+00 5.00e-01f  2
   8  9.8586451e-03 0.00e+00 1.15e+00  -1.7 1.10e-01    -  1.00e+00 1.00e+00f  1
   9  2.3237475e-03 0.00e+00 1.00e+00  -1.7 1.00e-01    -  1.00e+00 1.00e+00f  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  10  2.3797236e-04 0.00e+00 2.19e-01  -1.7 5.09e-02    -  1.00e+00 1.00e+00f  1
  11  4.9267371e-06 0.00e+00 5.95e-02  -1.7 2.53e-02    -  1.00e+00 1.00e+00f  1
  12  2.8189505e-09 0.00e+00 8.31e-04  -2.5 3.20e-03    -  1.00e+00 1.00e+00f  1
  13  1.0095040e-15 0.00e+00 8.68e-07  -5.7 9.78e-05    -  1.00e+00 1.00e+00f  1
  14  1.3288608e-28 0.00e+00 2.02e-13  -8.6 4.65e-08    -  1.00e+00 1.00e+00f  1

Number of Iterations...: 14

                                   (scaled)                 (unscaled)
Objective...:   1.3288608467480825e-28    1.3288608467480825e-28
Dual infeasibility...:   2.0183854587685121e-13    2.0183854587685121e-13
Constraint violation...:   0.0000000000000000e+00    0.0000000000000000e+00
Complementarity...:   0.0000000000000000e+00    0.0000000000000000e+00
Overall NLP error...:   2.0183854587685121e-13    2.0183854587685121e-13


Number of objective function evaluations             = 36
Number of objective gradient evaluations             = 15
Number of equality constraint evaluations            = 0
Number of inequality constraint evaluations          = 0
Number of equality constraint Jacobian evaluations   = 0
Number of inequality constraint Jacobian evaluations = 0
Number of Lagrangian Hessian evaluations             = 14
Total CPU secs in IPOPT (w/o function evaluations)   =      0.158
Total CPU secs in NLP function evaluations           =      0.024

EXIT: Optimal Solution Found.
x = 0.9999999999999899 y = 0.9999999999999792
```

In [31]:
```
# not bad, right?
# adding the constraint from before:

let

    m = Model(solver=IpoptSolver())

    @variable(m, x)
    @variable(m, y)
```

```
    @NLobjective(m, Min, (1-x)^2 + 100(y-x^2)^2)
    @NLconstraint(m,x^2 + y^2 <= 0.8)

    solve(m)

    println("x = ", getvalue(x), " y = ", getvalue(y))

  end
```

```
This is Ipopt version 3.12.8, running with linear solver mumps.
NOTE: Other linear solvers might be more efficient (see Ipopt documentation).

Number of nonzeros in equality constraint Jacobian...:        0
Number of nonzeros in inequality constraint Jacobian.:        2
Number of nonzeros in Lagrangian Hessian...:        5

Total number of variables...:        2
                     variables with only lower bounds:        0
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints...:        0
Total number of inequality constraints...:        1
        inequality constraints with only lower bounds:        0
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        1

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0  1.0000000e+00 0.00e+00 2.00e+00  -1.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1  9.5312500e-01 0.00e+00 1.25e+01  -1.0 5.00e-01    -  1.00e+00 5.00e-01f  2
   2  4.9204994e-01 0.00e+00 9.72e-01  -1.0 8.71e-02    -  1.00e+00 1.00e+00f  1
   3  2.0451702e+00 0.00e+00 3.69e+01  -1.7 3.80e-01    -  1.00e+00 1.00e+00H  1
   4  1.0409466e-01 0.00e+00 3.10e-01  -1.7 1.46e-01    -  1.00e+00 1.00e+00f  1
   5  8.5804626e-02 0.00e+00 2.71e-01  -1.7 9.98e-02    -  1.00e+00 1.00e+00h  1
   6  9.4244879e-02 0.00e+00 6.24e-02  -1.7 3.74e-02    -  1.00e+00 1.00e+00h  1
   7  8.0582034e-02 0.00e+00 1.51e-01  -2.5 6.41e-02    -  1.00e+00 1.00e+00h  1
   8  7.8681242e-02 0.00e+00 2.12e-03  -2.5 1.12e-02    -  1.00e+00 1.00e+00h  1
   9  7.6095770e-02 0.00e+00 6.16e-03  -3.8 1.37e-02    -  1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  10  7.6033892e-02 0.00e+00 2.23e-06  -3.8 3.99e-04    -  1.00e+00 1.00e+00h  1
  11  7.5885642e-02 0.00e+00 2.07e-05  -5.7 7.99e-04    -  1.00e+00 1.00e+00h  1
  12  7.5885428e-02 0.00e+00 2.74e-11  -5.7 1.38e-06    -  1.00e+00 1.00e+00h  1
  13  7.5883585e-02 0.00e+00 3.19e-09  -8.6 9.93e-06    -  1.00e+00 1.00e+00f  1

Number of Iterations...: 13

                                   (scaled)                 (unscaled)
Objective...:   7.5883585442440671e-02    7.5883585442440671e-02
```

```
Dual infeasibility...:   3.1949178858070582e-09    3.1949178858070582e-09
Constraint violation...:   0.0000000000000000e+00    0.0000000000000000e+00
Complementarity...:   2.5454985882932001e-09    2.5454985882932001e-09
Overall NLP error...:   3.1949178858070582e-09    3.1949178858070582e-09


Number of objective function evaluations             = 20
Number of objective gradient evaluations             = 14
Number of equality constraint evaluations            = 0
Number of inequality constraint evaluations          = 20
Number of equality constraint Jacobian evaluations   = 0
Number of inequality constraint Jacobian evaluations = 14
Number of Lagrangian Hessian evaluations             = 13
Total CPU secs in IPOPT (w/o function evaluations)   =      0.005
Total CPU secs in NLP function evaluations           =      0.003

EXIT: Optimal Solution Found.
x = 0.7247018392092258 y = 0.5242206029480763
```

2.14 JuMP: Maximium Likelihood

- Let's redo the maximum likelihood example in JuMP.
- Let μ, σ^2 be the unknown mean and variance of a random sample generated from the normal distribution.
- Find the maximum likelihood estimator for those parameters!
- density:

$$f(x_i|\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x_i-\mu)^2}{2\sigma^2}\right)$$

- Likelihood Function

$$\begin{aligned} L(\mu,\sigma^2) = \Pi_{i=1}^N f(x_i|\mu,\sigma^2) &= \frac{1}{(\sigma\sqrt{2\pi})^n} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^N (x_i-\mu)^2\right) \\ &= \left(\sigma^2 2\pi\right)^{-\frac{n}{2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^N (x_i-\mu)^2\right) \end{aligned}$$

- Constraints: $\mu \in \mathbb{R}, \sigma > 0$
- log-likelihood:

$$\log L = l = -\frac{n}{2}\log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\sum_{i=1}^N (x_i-\mu)^2$$

- Let's do this in `JuMP`.

```
In [32]: #  Copyright 2015, Iain Dunning, Joey Huchette, Miles Lubin, and contributors
         #  example modified
         using Distributions

         let
             distrib = Normal(4.5,3.5)
             n = 10000

             data = rand(distrib,n);

             m = Model(solver=IpoptSolver())

             @variable(m, mu, start = 0.0)
             @variable(m, sigma >= 0.0, start = 1.0)

             @NLobjective(m, Max, -(n/2)*log(2*sigma^2)-sum((data[i] - mu) ^ 2 for i = 1:n)/(2*s

             solve(m)
             println(" = ", getvalue(mu),", mean(data) = ", mean(data))
             println("^2 = ", getvalue(sigma)^2, ", var(data) = ", var(data))
         end
```

```
This is Ipopt version 3.12.8, running with linear solver mumps.
NOTE: Other linear solvers might be more efficient (see Ipopt documentation).

Number of nonzeros in equality constraint Jacobian...:        0
Number of nonzeros in inequality constraint Jacobian.:        0
Number of nonzeros in Lagrangian Hessian...:        3

Total number of variables...:        2
                     variables with only lower bounds:        1
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints...:        0
Total number of inequality constraints...:        0
        inequality constraints with only lower bounds:        0
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0  1.7210445e+05 0.00e+00 1.01e+02  -1.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1  1.2939451e+05 0.00e+00 1.07e+02  -1.0 9.80e+00    -  1.00e+00 5.00e-01f  2
   2  7.8864616e+04 0.00e+00 4.43e+01  -1.0 2.27e-01    -  8.88e-01 1.00e+00f  1
   3  5.1720095e+04 0.00e+00 1.84e+01  -1.0 2.96e-01    -  1.00e+00 1.00e+00f  1
   4  3.7648943e+04 0.00e+00 7.44e+00  -1.0 3.75e-01    -  1.00e+00 1.00e+00f  1
   5  3.0796009e+04 0.00e+00 2.93e+00  -1.0 4.57e-01    -  1.00e+00 1.00e+00f  1
   6  2.7858621e+04 0.00e+00 1.07e+00  -1.0 5.13e-01    -  1.00e+00 1.00e+00f  1
   7  2.6886136e+04 0.00e+00 3.39e-01  -1.0 4.94e-01    -  1.00e+00 1.00e+00f  1
```

```
   8  2.6711082e+04 0.00e+00 6.36e-02  -1.7 3.19e-01    -  1.00e+00 1.00e+00f  1
   9  2.6701110e+04 0.00e+00 4.25e-03  -2.5 1.01e-01    -  1.00e+00 1.00e+00f  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  10  2.6701072e+04 0.00e+00 1.72e-05  -3.8 6.78e-03    -  1.00e+00 1.00e+00f  1
  11  2.6701072e+04 0.00e+00 8.12e-10  -5.7 4.62e-05    -  1.00e+00 1.00e+00f  1
  12  2.6701072e+04 0.00e+00 4.04e-13  -8.6 1.02e-06    -  1.00e+00 1.00e+00f  1

Number of Iterations...: 12

                                   (scaled)                 (unscaled)
Objective...:   8.4542511167531504e+00    2.6701072346234618e+04
Dual infeasibility...:   4.0444162230182163e-13    1.2773485040573046e-09
Constraint violation...:   0.0000000000000000e+00    0.0000000000000000e+00
Complementarity...:   2.5064398796454131e-09    7.9160923461665668e-06
Overall NLP error...:   2.5064398796454131e-09    7.9160923461665668e-06


Number of objective function evaluations             = 18
Number of objective gradient evaluations             = 13
Number of equality constraint evaluations            = 0
Number of inequality constraint evaluations          = 0
Number of equality constraint Jacobian evaluations   = 0
Number of inequality constraint Jacobian evaluations = 0
Number of Lagrangian Hessian evaluations             = 12
Total CPU secs in IPOPT (w/o function evaluations)   =      0.007
Total CPU secs in NLP function evaluations           =      0.026

EXIT: Optimal Solution Found.
 = 4.513536352090578, mean(data) = 4.513536352090578
^2 = 12.211002671496686, var(data) = 12.212223884224223
```

3 Linear Constrained Problems (LPs)

- Very similar to before, just that both objective and constraints are *linear*.

$$
\begin{aligned}
\min_{\mathbf{x}} \mathbf{c}^T\mathbf{x} \\
\text{subject to } \mathbf{w}_{LE}^{(i)T}\mathbf{x} \leq b_i \text{ for } i \in 1,2,3,\ldots \\
\mathbf{w}_{GE}^{(j)T}\mathbf{x} \geq b_j \text{ for } j \in 1,2,3,\ldots \\
\mathbf{w}_{EQ}^{(k)T}\mathbf{x} = b_k \text{ for } k \in 1,2,3,\ldots
\end{aligned}
$$

3.0.1 Standard Form

- Usually LPs are given in *standard form*
- All constraints are less-than inequalities

- All choice variables are non-negative.

$$\min_{\mathbf{x}} \mathbf{c}^T \mathbf{x}$$
$$\text{subject to } \mathbf{A}\mathbf{x} \leq b$$
$$\mathbf{x} \geq 0$$

- Greater-than inequality constraints are inverted
- equality constraints are split into two
- $\mathbf{x} = \mathbf{x}^+ - \mathbf{x}^-$ and we constrain both components to be positive.

3.0.2 Equality Form

$$\min_{\mathbf{x}} \mathbf{c}^T \mathbf{x}$$
$$\text{subject to } \mathbf{A}\mathbf{x} = b$$
$$\mathbf{x} \geq 0$$

- Can transform standard into equality form

$$\mathbf{A}\mathbf{x} \leq b \rightarrow \mathbf{A}\mathbf{x} + \mathbf{s} = b, \mathbf{s} \geq 0$$

- equality constraints are split into two
- $\mathbf{x} = \mathbf{x}^+ - \mathbf{x}^-$ and we constrain both components to be positive.

3.0.3 Solving LPs

- Simplex Algorithm operates on Equality Form
- Moving from one vertex to the next of the feasible set, this is guaranteed to find the optimal solution if the problem is bounded.

4 Discrete Optimization / Integer Programming

- Here the choice variable is contrained to come from a discrete set $\mathcal{X}$.
- If this set is $\mathcal{X} = \mathbb{N}$, we have an **integer program**
- If only *some* x have to be discrete, this is a **mixed integer program**

4.1 Example

$$\min_{\mathbf{x}} x_1 + x_2$$
$$\text{subject to } ||\mathbf{x}|| \leq 2$$
$$\mathbf{x} \in \mathbb{N}$$

- continuous optimum is $(-\sqrt{2}, -\sqrt{2})$ and objective is $y = -2\sqrt{2} = -2.828$
- Integer constrained problem is only delivering $y = -2$, and $\mathbf{x}^* \in (-2, 0), (-1, -1), (0, -2)$

```
In [33]: x = -3:0.01:3
         dx = repmat(linspace(-3,3,7),1,7)
         contourf(x,x,(x,y)->x+y,color=:blues)
         scatter!(dx,dx',legend=false,markercolor=:white)
         plot!(x->sqrt(4-x^2),-2,2,c=:white)
         plot!(x->-sqrt(4-x^2),-2,2,c=:white)
         scatter!([-2,-1,0],[0,-1,-2],c=:red)
         scatter!([-sqrt(2)],[-sqrt(2)],c=:red,markershape=:cross,markersize=9)
```

4.2 Rounding

- One solution is to just *round the continuous solution to the nearest integer*
- We compute the **relaxed** problem, i.e. the one where x is continuous.
- Then we round up or down.
- Can go terribly wrong.

4.3 Cutting Planes

- This is an exact method
- We solve the relaxed problem first.
- Then we add linear constraints that result in the solution becoming integral.

4.4 Branch and Bound

- This enumerates all possible soultions.
- Branch and bound does this, without having to compute all of them.

4.5 Example: The Knapsack Problem

- We are packing our knapsack for a trip but only have space for the most valuable items.
- We have $x_i = 0$ if item i is not in the sack, 1 else.

$$\min_x - \sum_{i=1}^n v_i x_i$$
$$\text{s.t.} \sum_{i=1}^n w_i x_i \leq w_{max}$$
$$w_i \in \mathbb{N}_+, v_i \in \mathbb{R}$$

- If ther are n items, we have 2^n possible design vectors.
- But there is a useful recursive relationship.
- If we solved $n-1$ knapsack problems so far and deliberate about item n
  - If it's not worth including item n, then the solution **is** the knapsack problem for $n-1$ items and capacity w_{max}
  - If it IS worth including it: solution will have value of knapsack with $n-1$ items and reduced capacity, plus the value of the new item

In [34]:
```julia
#  Copyright 2017, Iain Dunning, Joey Huchette, Miles Lubin, and contributors
#  This Source Code Form is subject to the terms of the Mozilla Public
#  License, v. 2.0. If a copy of the MPL was not distributed with this
#  file, You can obtain one at http://mozilla.org/MPL/2.0/.
#############################################################################
# JuMP
# An algebraic modeling langauge for Julia
# See http://github.com/JuliaOpt/JuMP.jl
#############################################################################
# knapsack.jl
#
# Solves a simple knapsack problem:
# max sum(p_j x_j)
#  st sum(w_j x_j) <= C
#     x binary
#############################################################################

using JuMP, Cbc

let

    # Maximization problem
    m = Model(solver=CbcSolver())

    @variable(m, x[1:5], Bin)

    profit = [ 5, 3, 2, 7, 4 ]
    weight = [ 2, 8, 4, 2, 5 ]
    capacity = 10

    # Objective: maximize profit
    @objective(m, Max, dot(profit, x))

    # Constraint: can carry all
    @constraint(m, dot(weight, x) <= capacity)

    # Solve problem using MIP solver
    status = solve(m)

    println("Objective is: ", getobjectivevalue(m))
    println("Solution is:")
    for i = 1:5
        print("x[$i] = ", getvalue(x[i]))
        println(", p[$i]/w[$i] = ", profit[i]/weight[i])
    end
end
```

```
Objective is: 16.0
```

```
Solution is:
x[1] = 1.0, p[1]/w[1] = 2.5
x[2] = 0.0, p[2]/w[2] = 0.375
x[3] = 0.0, p[3]/w[3] = 0.5
x[4] = 1.0, p[4]/w[4] = 3.5
x[5] = 1.0, p[5]/w[5] = 0.8
```