Constrained Optimization

Basic topics and examples using Julia Julia v1.5.3

Ricardo A. Fernandes

ricardoaf@lccv.ufal.br

Advisor: Adeildo S. Ramos Jr.







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Introduction

General optimization problem equation

subject to
$$x \in \mathcal{X}$$

Unconstrained problems:

• Feasible set χ is \mathbb{R}^n

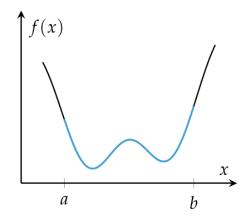
Constrained problems:

- Feasible set: subset of \mathbb{R}^n
- Design points must satisfy certain <u>conditions</u>

Bracketing constraints

Some constraints are simply <u>upper or lower bounds</u> on design variables

Univariate problem

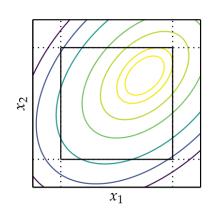


minimize f(x) subject to $x \in [a, b]$

Inequality constraints

- $x \ge a$
- *x* ≤ *b*

Multivariate problems



Solution must lie within a hyperrectangle

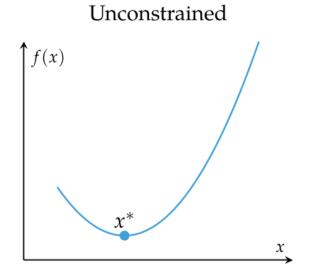
Introduction

Constrained problems

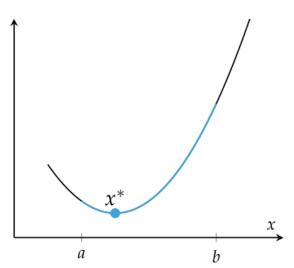
- Constraints arise naturally when formulating real problems
 - A structure dimension can't exceed a certain design limit
 - A fund manager can't sell more stock than they have
 - Number of hours spend per day on your job can't exceed X
 - In Sudoku, one can't repeat the same number within a row, column or block
- Constraints are included to prevent infeasible solutions



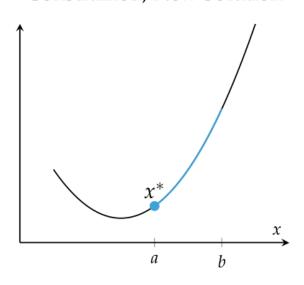
Applying constrains can affect the solution, or not







Constrained, New Solution



Constraint Types

The two constraint types

- The feasible set is typically formed from:
 - Equality constraints, h(x) = 0
 - Inequality constraints, $g(x) \le 0$

Greater-than inequalities $G(x) \ge 0$ can be translated as $-G(x) \le 0$

Using set membership (not typical)

 $\bullet \quad h(x) = (x \notin \chi)$

Using functions

- $h(x) = 0, g(x) \le 0$
- Functions are often used because they can provide information about how far a given point is from being feasible, helping drive solution methods

Any optimization problem can be rewritten like:

minimize
$$f(\mathbf{x})$$

subject to $h_i(\mathbf{x}) = 0$ for all i in $\{1, \dots, \ell\}$
 $g_j(\mathbf{x}) \leq 0$ for all j in $\{1, \dots, m\}$

Equality constraint as two inequality constraints

$$h(\mathbf{x}) = 0 \iff \begin{cases} h(\mathbf{x}) \le 0 \\ h(\mathbf{x}) \ge 0 \end{cases}$$

Transformations: Removing Constraints

Problem transformation

- Removing constraints
- Such transformations may be possible in some cases

Eliminating design variables

Consider the equality constraint

$$h(x) = \alpha_1 x_1 + \alpha_2 x_2 + \dots + \alpha_n x_n - \beta = 0$$

• x_n can solved using the first n-1 variables

$$x_n = 1/\alpha_n [\beta - \alpha_1 x_1 - \alpha_2 x_2 - \dots - \alpha_{n-1} x_{n-1}]$$

So, one can transform the problem

minimize
$$f(x)$$

s.t. $h(x) = 0$ into

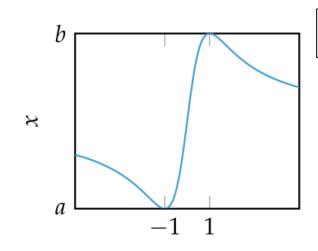
minimize
$$f(x_1, ..., x_{n-1})$$

with $x_n = 1/\alpha_n[\beta - \alpha_1 x_1 - \alpha_2 x_2 - \cdots - \alpha_{n-1} x_{n-1}]$

Removing bound constraints

■ Bound constraints $a \le x \le b$ can be removed

$$x = t_{a,b}(\hat{x}) = \frac{b+a}{2} + \frac{b-a}{2} \left(\frac{2\hat{x}}{1+\hat{x}^2}\right)$$



This transformation ensures that $a \le x \le b$

Transformations: Removing Constraints

Example: Removing bound constraints

Kochenderfer & Wheeler (2019) Algorithms for Optimization, MIT Press: Example 10.1 (page 170)

Consider the following optimization problem

minimize
$$x \sin(x)$$

subject to $2 \le x \le 6$

Transformation

$$x = t_{a,b}(\hat{x}) = \frac{b+a}{2} + \frac{b-a}{2} \left(\frac{2\hat{x}}{1+\hat{x}^2}\right)$$

Problem can be transformed into

minimize
$$t_{2,6}(\hat{x})\sin(t_{2,6}(\hat{x}))$$
minimize $\left(4+2\left(\frac{2\hat{x}}{1+\hat{x}^2}\right)\right)\sin\left(4+2\left(\frac{2\hat{x}}{1+\hat{x}^2}\right)\right)$

- One can solve the unconstrained problem
 - two minimum values can be found

•
$$\hat{x} \approx 0.242, \ \hat{x} \approx 4.139$$

• both values of \hat{x} produce

•
$$x = t_{2.6}(\hat{x}) = 4.914$$

■ an objective function value of \approx -4.814

Optimization problem with bound constraints

```
In [1]: using Optim, Plots
In [2]: # Objective function
f(x) = x * sin(x)
# Design variable bounds
xmin, xmax = 2., 6.;
```

Constrained Optimization

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```
In [3]: # Constrained optimization
         function constrainedOptimization(f, xmin, xmax)
             res = optimize(f, xmin, xmax)
             conv = Optim.converged(res); println("converged? ", conv)
xopt = Optim.minimizer(res); println(" xOpt: ", xopt)
             fmin = Optim.minimum(res); println("
                                                             fMin: ", fmin)
             xopt, fmin
In [4]: # Perform constrained optimization
         xopt, fmin = constrainedOptimization(f, xmin, xmax)
         # pLot
         plot(f, 0, xmin, color=:black, title="f(x)", xlabel="x", legend=false)
         plot!(f, xmin, xmax, color=:blue, linewidth=5)
         plot!(f, xmax, 15, color=:black)
         scatter!([xopt], [fmin], color=:white, markersize=5)
         converged? true
            # iter: 10
              xOpt: 4.913180438706312
               fMin: -4,814469889712268
Out[4]:
                                                   f(x)
```

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Unconstrained Optimization (transformed problem)

```
# Transformation
 x(y) = 0. (xmin + xmax) / 2 + (xmax - xmin) * y / (1 + y^2)
fy(y) = f(x(y))
# Unconstrained optimization: transformed problem
function unconstrainedOptimization(fy, y0, method=LBFGS())
    println("\ninitial guess: ", y0)
    res = optimize(y->fy(first(y)), [y0], method)
    conv = Optim.converged(res); println("converged? ",
    yopt = Optim.minimizer(res); println("
                                                           yopt[1])
                                  println("
                                                xOpt: ", x(yopt[1]))
                                                fMin: ",
    fmin = Optim.minimum(res);
                                  println("
    yopt, fmin
end:
```

```
# Perform constrained optimization

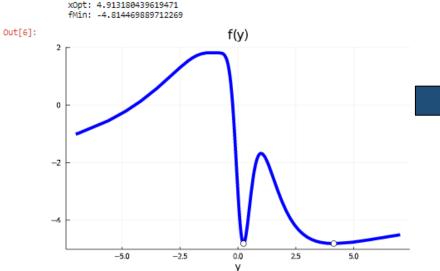
# different initial guesses
yopt_a, fmin_a = unconstrainedOptimization(fy, 0.)
yopt_b, fmin_b = unconstrainedOptimization(fy, 0.5)

# plot
plot(fy, -7, 7, color=:blue, linewidth=5, title="f(y)", xlabel="y", legend=false)
scatter!([yopt_a], [fmin_a], color=:white, markersize=5)
scatter!([yopt_b], [fmin_b], color=:white, markersize=5)

initial guess: 0.0
converged? true
    yopt: 4.138671948497414
    xOpt: 4.913180431692558
fMin: -4.814469889712268
```

Optim

https://julianlsolvers.github.io/Optim.jl/stable/



initial guess: 0.5

yOpt: 0.24162340533417573

converged? true



See 01 alg4opt170.ipynb

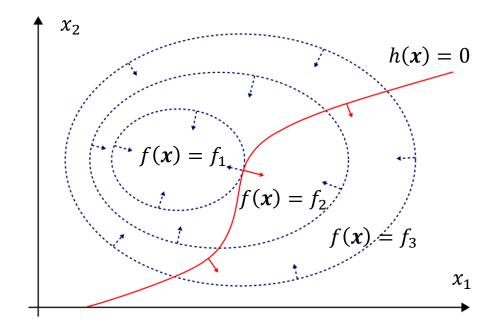
Method of Lagrange Multipliers

Used to optimize a function subjected to equality constraints

Consider an optimization problem where f and h have continuous partial derivatives

minimize
$$f(\mathbf{x})$$
 subject to $h(\mathbf{x}) = 0$

- Method of Lagrange multipliers is used to compute where a contour line of f is aligned with a contour line of h=0
- Hence, we need to find where the gradient of f and the gradient of h are aligned



- Contour lines of f are lines of constant f
- The gradient of a function at a point is perpendicular to the contour line of that function through that point
- The optimum solution x^* lies where a contour line of f is align with the contour line h=0

Example: Aligned gradients

Kochenderfer & Wheeler (2019) Algorithms for Optimization, MIT Press: Example 10.3 (page 172)

minimize
$$-\exp\left(-\left(x_1x_2 - \frac{3}{2}\right)^2 - (x_2 - \frac{3}{2})^2\right)$$
 subject to
$$x_1 - x_2^2 = 0$$

Lagrange Multiplier Motivation

Otimization problem with equality constraint

```
In [1]: using Optim, Calculus, LinearAlgebra, Plots
In [2]: # Objective function
f(x) = -exp(-(x[1] * x[2] - 3/2)^2 - (x[2]- 3 /2)^2)
# Equality constraint
h(x) = x[1] - x[2]^2;
```

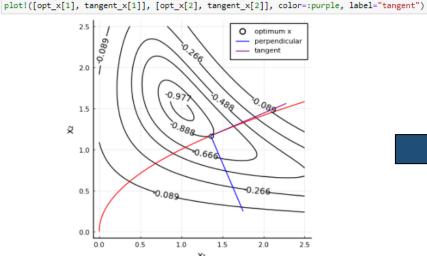
Find optimal solution

Alignment of gradients

In [4]: # Objective and constraint gradients

```
∇f = Calculus.gradient(f)
         ∇h = Calculus.gradient(h);
In [5]: # eval gradients at optimal point
         nf = normalize!(\nabla f(opt_x))
         nh = normalize!(\nabla h(opt x));
         println("nf: ", nf)
         println("nh: ", nh)
         nf: [0.3943241793241729, -0.918971404125459]
         nh: [0.39432418041471096, -0.9189714036575167]
In [6]: # plots
         pyplot(xlabel="x1", ylabel="x2", colorbar=false, aspect_ratio=:equal)
         x = y = LinRange(0, 2.5, 100)
         contour(x, y, (x, y)->f([x, y]), levels=[1.1, 1, 0.75, 0.55, 0.3, 0.1]*min_f, c=:black, contour_labels=true)
         contour!(x, y, (x, y)\rightarrow h([x, y]), levels=[0.], c=:red)
         scatter!([x<sub>1</sub>(opt_x<sub>2</sub>)], [opt_x<sub>2</sub>], markersize=5, c=:white, label="optimum x")
         perpend x = opt x + nh
         tangent_x = opt_x + [-nh[2], nh[1]]
```

Out[6]:



plot!([opt_x[1], perpend_x[1]], [opt_x[2], perpend_x[2]], color=:blue, label="perpendicular")



See 02 lagmul.ipynb

Method of Lagrange Multipliers

So, we seek the best \boldsymbol{x} such that

- h(x) = 0

Lagrange multiplier, λ

• We need the scalar λ because the magnitudes of the gradients may not be the same

We can formulate the Lagrangian as

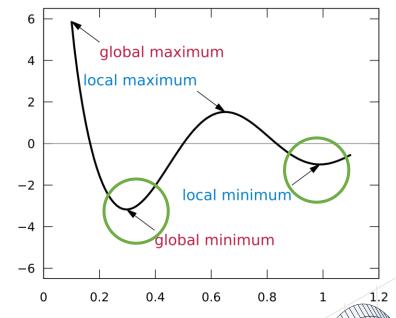
•
$$\mathcal{L}(x,\lambda) = f(x) - \lambda h(x)$$

Solving $\nabla \mathcal{L}(\mathbf{x}, \lambda) = \mathbf{0}$

•
$$\nabla_{\mathbf{x}} \mathcal{L} = \mathbf{0} \implies \nabla f(\mathbf{x}) = \lambda \, \nabla h(\mathbf{x})$$

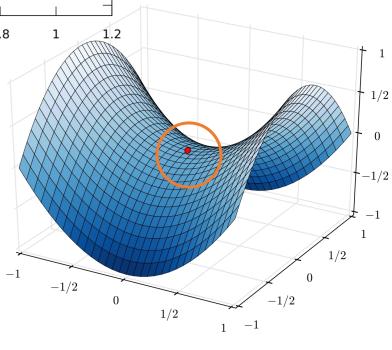
Any solution is considered a *critical point*

- Local/global minimum
- Saddle points



Necessary optimally conditions (not sufficient)

For convex problems, Necessary conditions = sufficient conditions



Consider the same last example

minimize
$$-\exp\left(-\left(x_1x_2 - \frac{3}{2}\right)^2 - (x_2 - \frac{3}{2})^2\right)$$
 subject to
$$x_1 - x_2^2 = 0$$

Form the Lagrangian

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

Compute the gradient and set the derivatives to zero

$$\frac{\partial \mathcal{L}}{\partial x_1} = 2x_2 f(\mathbf{x}) \left(\frac{3}{2} - x_1 x_2 \right) - \lambda$$

$$\frac{\partial \mathcal{L}}{\partial x_2} = 2\lambda x_2 + f(\mathbf{x}) \left(-2x_1 (x_1 x_2 - \frac{3}{2}) - 2(x_2 - \frac{3}{2}) \right)$$

$$\frac{\partial \mathcal{L}}{\partial \lambda} = x_2^2 - x_1$$

- Solve equations and the same solution is obtained:
 - $x_1 \approx 1.358, x_2 \approx 1.165$
 - with Lagrange multiplier, $\lambda \approx 0.170$

Lagrange Multipliers for multiple equality constraints

Consider the following optimization problem

minimize
$$f(\mathbf{x})$$

subject to $h_1(\mathbf{x}) = 0$
 $h_2(\mathbf{x}) = 0$
 \vdots

Lagrangian can be defined as

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) - \sum_{i} \lambda_{i} h_{i}(\mathbf{x})$$
$$= f(\mathbf{x}) - \boldsymbol{\lambda}^{T} h(\mathbf{x})$$

Example: Minimization of Complementary Energy

Optimization problem

$$\min_{\boldsymbol{r}} \operatorname{minimize} \quad \Pi_{c}(\boldsymbol{r})$$

s.t.
$$\mathbf{B}^T \mathbf{r} = \mathbf{f}$$

Complementary Energy

$$\Pi_c(\mathbf{r}) = \frac{1}{2} \, \mathbf{r}^T \, \mathbf{F} \, \mathbf{r}$$

where:

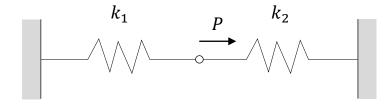
r: Internal forces of the bars

f: Nodal external forces

 $\boldsymbol{B^T}$: Equilibrium matrix

F: Flexibility matrix

Example: Minimization of Complementary Energy



Equilibrium condition (internal x external forces)

$$r_1 \xrightarrow{P} r_2$$
 $r_2 - r_1 = P$

Complementary Energy

$$\Pi_c(r_1, r_2) = \frac{1}{2} \frac{r_1^2}{k_1} + \frac{1}{2} \frac{r_2^2}{k_2}$$

Optimization Problem

minimize
$$\Pi_c(r_1, r_2)$$

s.t. $r_2 - r_1 = P$

Complementary Energy Example

Complementary Energy and Equilibrium Condition

$$\Pi_c := (r_1, r_2) \to \frac{1}{2} \cdot \frac{1}{k_1} \cdot r_1^2 + \frac{1}{2} \cdot \frac{1}{k_2} \cdot r_2^2 :$$

$$h := (r_1, r_2) \to r_2 - r_1 + P :$$

using Force method

$$r2 := solve(h(r_1, r_2) = 0, r_2) = r_1 - P$$

$$r_1^2 \qquad (r_1 - P)^2$$

$$\Pi_c(r_1, r_2) = \frac{r_I^2}{2 k_I} + \frac{(r_I - P)^2}{2 k_2}$$

$$r1 := solve(diff(\Pi_c(r_1, r_2), r_1) = 0, r_1) = \frac{P k_1}{k_2 + k_1}$$

$$r2 := solve(h(r1, r_2) = 0, r_2) = -\frac{P k_2}{k_2 + k_1}$$

using Lagrange multiplier

$$L := (r_1, r_2, \lambda) \rightarrow \Pi_c(r_1, r_2) + \lambda \cdot h(r_1, r_2) :$$

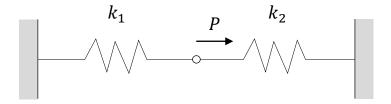
$$eq_1 := diff(L(r_1, r_2, \lambda), r_1) = 0 = \frac{r_1}{k_1} - \lambda = 0$$

$$eq_2 := diff(L(r_1, r_2, \lambda), r_2) = 0 = \frac{r_2}{k_2} + \lambda = 0$$

$$eq_3 := diff(L(r_1, r_2, \lambda), \lambda) = 0 = r_2 - r_1 + P = 0$$

$$solve(\{eq_1, eq_2, eq_3\}, \{r_1, r_2, \lambda\}) = \left\{\lambda = \frac{P}{k_2 + k_1}, r_1 = \frac{P k_1}{k_2 + k_1}, r_2 = -\frac{P k_2}{k_2 + k_1}\right\}$$

Example: Minimization of Complementary Energy



Equilibrium condition (internal x external forces)

$$r_1 \xrightarrow{P} r_2$$
 $r_2 - r_1 = P$

Complementary Energy

$$\Pi_c(r_1, r_2) = \frac{1}{2} \frac{r_1^2}{k_1} + \frac{1}{2} \frac{r_2^2}{k_2}$$

Optimization Problem

minimize
$$\Pi_c(r_1, r_2)$$

s.t. $r_2 - r_1 = P$

Complementary Energy Example

```
In [1]: using JuMP, Ipopt
In [2]: # Problem data
        P, k_1, k_2 = 10., 100., 200.
        # Complementary energy and equilibrium condition
        \Pi c(r_1, r_2) = 1/2 * r_1^2 / k_1 + 1/2 * r_2^2 / k_2
         h(r_1, r_2) = r_2 - r_1 + P;
        # reference results
        r_1ref(P, k_1, k_2) = P * k_1 / (k_1 + k_2)
        r_2ref(P, k_1, k_2) = -P * k_2 / (k_1 + k_2)
        println("r_1ref : ", r_1ref(P, k_1, k_2), ", r_2ref : ", r_2ref(P, k_1, k_2))
        r<sub>1</sub>ref : 3.333333333333335, r<sub>2</sub>ref : -6.6666666666666667
In [3]: m = Model(Ipopt.Optimizer)
        set optimizer attribute(m, "print level", 0)
        @variable(m, r<sub>1</sub>)
        @variable(m, r2)
        @objective(m, Min, ∏c(r₁, r₂))
        @constraint(m, h(r_1, r_2) == 0)
                                                              See 03 complementaryenergy.ipynb
        println(m)
        optimize!(m)
        println("Termination status: ", termination status(m))
        println("Primal status: ", primal_status(m))
        println(" f* : ", objective value(m))
        println("r_1* : ", value(r_1), ", r_2* : ", value(r_2))
        Min 0.005 r_1^2 + 0.0025 r_2^2
        Subject to
         -r_1 + r_2 == -10.0
        ****************************
        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
        ****************************
        Termination status: LOCALLY SOLVED
        Primal status: FEASIBLE POINT
        f*: 0.1666666666666669
        r_1^*: 3.333333333333335, r_2^*: -6.666666666666667
```

About JuMP solvers

JuMP depends on solvers to solve optimization problems

https://jump.dev/JuMP.jl/v0.21.1/installation/#Getting-Solvers-1

Solver	Julia Package	License	Supports
Artelys Knitro	KNITRO.jI	Comm.	LP, MILP, SOCP, MISOCP, NLP, MINLP
Cbc	Cbc.jl	EPL	MILP
CDCS	CDCS.jl	GPL	LP, SOCP, SDP
CDD	CDDLib.jl	GPL	LP
Clp	Clp.jl	EPL	LP
COSMO	COSMO.jI	Apache	LP, QP, SOCP, SDP
CPLEX	CPLEX.jl	Comm.	LP, MILP, SOCP, MISOCP
CSDP	CSDP.jI	EPL	LP, SDP
ECOS	ECOS.jl	GPL	LP, SOCP
FICO Xpress	Xpress.jl	Comm.	LP, MILP, SOCP, MISOCP
GLPK	GLPK.jl	GPL	LP, MILP
Gurobi	Gurobi.jl	Comm.	LP, MILP, SOCP, MISOCP
Ipopt	lpopt.jl	EPL	LP, QP, NLP

Juniper	Juniper.jl	MIT	MISOCP, MINLP
MOSEK	MosekTools.jl	Comm.	LP, MILP, SOCP, MISOCP, SDP
OSQP	OSQP.jI	Apache	LP, QP
ProxSDP	ProxSDP.jl	MIT	LP, SOCP, SDP
SCIP	SCIP.jl	ZIB	MILP, MINLP
SCS	SCS.jl	MIT	LP, SOCP, SDP
SDPA	SDPA.jl, SDPAFamily.jl	GPL	LP, SDP
SDPNAL	SDPNAL.jI	CC BY-SA	LP, SDP
SDPT3	SDPT3.jl	GPL	LP, SOCP, SDP
SeDuMi	SeDuMi.jI	GPL	LP, SOCP, SDP
Tulip	Tulip.jl	MPL-2	LP

Where:

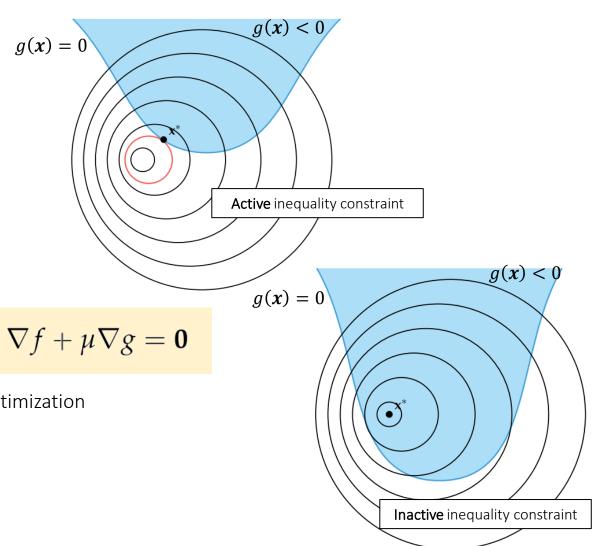
- LP = Linear programming
- QP = Quadratic programming
- SOCP = Second-order conic programming (including problems with convex quadratic constraints and/or objective)
- MILP = Mixed-integer linear programming
- NLP = Nonlinear programming
- MINLP = Mixed-integer nonlinear programming
- SDP = Semidefinite programming
- MISDP = Mixed-integer semidefinite programming

Inequality constraints

Consider a problem with a single inequality constraint

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

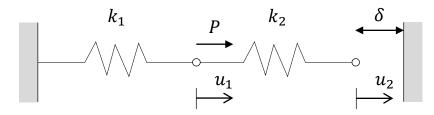
- If the solution <u>lies</u> at the constraint boundary,
 - the Lagrange condition holds for some constant μ
 - the constraint is considered active
- If the solution <u>does not lie</u> at the constraint boundary,
 - the constraint is considered inactive
 - solutions will lie where $\nabla f = 0$, as with unconstrained optimization
 - the Lagrange condition holds by setting $\mu = 0$
- The Lagrangian of the problem is $\mathcal{L}(x,\mu) = f(x) + \mu g(x)$
- In order to penalize the objective, for inequalities $\mu \geq 0$



Total Potential Energy

$$\Pi(\boldsymbol{u}) = \frac{1}{2} \, \boldsymbol{u}^T \, \boldsymbol{K} \, \boldsymbol{u} \, - \boldsymbol{f}^T \, \boldsymbol{u}$$

Example: Contact Problem



Contact condition

$$u_2 \leq \delta$$

Optimization Problem

minimize
$$\Pi(u_1, u_2) = \frac{1}{2}k_1u_1^2 + \frac{1}{2}k_2(u_2 - u_1)^2 - Pu_1$$

s.t. $u_2 - \delta \le 0$

Contact Problem

restart: with(LinearAlgebra):

Set stiffness matrix

$$K := \langle k_1 + k_2 - k_2 - k_2, k_2 \rangle :$$

Approach #1: Solving linear system, Ku = f

Unconstrained problem

$$F := \langle P, 0 \rangle :$$

$$u := LinearSolve(K, F) :$$

$$u^{\%T} = \left[\begin{array}{c} \frac{P}{k_1} & \frac{P}{k_1} \end{array} \right]$$

Constrained problem

$$u := \langle 0, \delta \rangle$$
: free := 1: fix := 2:

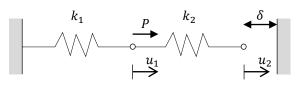
Apply partition method for solving the unknowns

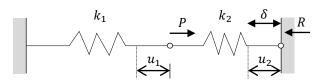
$$u[free] := \frac{1}{K[free, free]} :$$

$$F[fix] := K[fix, free] \cdot u[free] + K[fix, fix] \cdot u[fix] :$$

$$u^{\%T} = \left[\frac{k_2 \delta + P}{k_1 + k_2} \delta \right]$$

$$F^{\%T} = \left[P \quad k_2 \delta - \frac{k_2 (k_2 \delta + P)}{k_1 + k_2} \right]$$

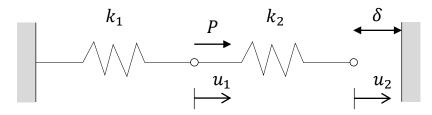




Total Potential Energy

$$\Pi(\boldsymbol{u}) = \frac{1}{2} \boldsymbol{u}^T \boldsymbol{K} \boldsymbol{u} - \boldsymbol{f}^T \boldsymbol{u}$$

Example: Contact Problem



Contact condition

$$u_2 \leq \delta$$

Optimization Problem

minimize
$$\Pi(u_1, u_2) = \frac{1}{2}k_1u_1^2 + \frac{1}{2}k_2(u_2 - u_1)^2 - Pu_1$$

s.t. $u_2 - \delta \le 0$

Approach #2: Solving a optimization problem

Total Potential Energy and Inequality constraint

$$\Pi := (u_1, u_2) \to \frac{1}{2} \cdot k_1 \cdot u_1^2 + \frac{1}{2} \cdot k_2 \cdot (u_2 - u_1)^2 - P \cdot u_1 :$$

$$g := (u_1, u_2) \to u_2 - \delta :$$

Lagrangian

$$L := unapply \left(\Pi(u_1, u_2) + \mu \cdot g(u_1, u_2), u_1, u_2, \mu \right) :$$

$$L(u_1, u_2, \mu) = \frac{k_1 u_1^2}{2} + \frac{k_2 (u_2 - u_1)^2}{2} - Pu_1 + \mu (u_2 - \delta)$$

Number of cases are 2^n , where n is the number of inequality constraints

Here, n=1, so the two cases are the unconstrained and the constrained cases

Unconstrained problem

Set Lagrange multiplier to zero (remove constraint from Lagrangian)

$$\begin{aligned} eq_1 &:= D[1](L) (u_1, u_2, 0) = k_1 u_1 - k_2 (u_2 - u_1) - P \\ eq_2 &:= D[2](L) (u_1, u_2, 0) = k_2 (u_2 - u_1) \\ solve(\{eq_1 = 0, eq_2 = 0\}, \{u_1, u_2\}) = \left\{u_1 = \frac{P}{k_1}, u_2 = \frac{P}{k_1}\right\} \end{aligned}$$

Constrained problem

Constraint g must be zero

$$u2 := solve(g(u_1, u_2) = 0, u_2) = \delta$$

$$eq_{1} := D[1](L)(u_{1}, u_{2}, \mu) = k_{1}u_{1} - k_{2}(\delta - u_{1}) - P$$

$$eq_{2} := D[2](L)(u_{1}, u_{2}, \mu) = k_{2}(\delta - u_{1}) + \mu$$

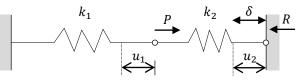
$$solve(\{eq_{1} = 0, eq_{2} = 0\}, \{u_{1}, \mu\}) = \left\{\mu = \frac{k_{2}(-\delta k_{1} + P)}{k_{1} + k_{2}}, u_{1} = \frac{k_{2}\delta + P}{k_{1} + k_{2}}\right\}$$

$$assign(\%):$$

Lagrange multiplier and reaction force

$$R := -F[2]:$$

 $simplify(R - \mu) = 0$

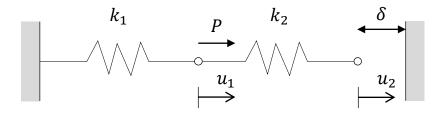


For inequality constraints, since $P - \delta \cdot k_1 \ge 0$, or reaction force due to contact is always non-negative, lagrange multiplier must always be non-negative too!

Total Potential Energy

$$\Pi(\boldsymbol{u}) = \frac{1}{2} \, \boldsymbol{u}^T \, \boldsymbol{K} \, \boldsymbol{u} \, - \boldsymbol{f}^T \, \boldsymbol{u}$$

Example: Contact Problem



Contact condition

$$u_2 \leq \delta$$

Optimization Problem

minimize
$$\Pi(u_1, u_2) = \frac{1}{2}k_1u_1^2 + \frac{1}{2}k_2(u_2 - u_1)^2 - Pu_1$$

s.t. $u_2 - \delta \le 0$

Given this optimization problem

Homework

- A) Consider:
 - P = 100 kN
 - $k_1 = k_2 = 1000 \text{ kN/m}$
 - $\delta = 0.15 \text{ m}$
 - Develop a computational routine to solve the problem
 - Verify the results with the analytical solution
- **B)** Repeat A) but now with P = 200 kN

Optimizing the problem

Requires finding critical points x^* such that

■ The point is feasible

$$g(\mathbf{x}^*) \leq 0$$

 $\mu \geq 0$

- The penalty must point in the right direction
- Active constraint, g(x) = 0
- Inactive constraint $\mu = 0$

$$\mu g(\mathbf{x}^*) = 0$$

- Active constraint, Lagrange condition holds
- Inactive constraint, optimum will have

 - $\mu = 0$

$$\nabla f(\mathbf{x}^*) + \mu \nabla g(\mathbf{x}^*) = \mathbf{0}$$

KKT Conditions

Generalizing for multiple equality and inequality constraints

Feasibility

All constraints satisfied

 $\mathbf{g}(\mathbf{x}^*) \leq \mathbf{0}$

 $\mathbf{h}(\mathbf{x}^*) = \mathbf{0}$

Dual feasibility

Penalization is toward feasibility

 $\mu \geq 0$

Complementary slackness

Either
$$\mu_i = 0$$
 or $g_i(x) = 0$

$$\mu_i g_i(\mathbf{x}^*) = 0$$

Stationarity

f contour is tangent to each active constraint

$$\nabla f(\mathbf{x}^*) + \sum_{i} \mu_i \nabla g_i(\mathbf{x}^*) + \sum_{j} \lambda_j \nabla h_j(\mathbf{x}^*) = \mathbf{0}$$

- First-order necessary conditions for optimality
- Identified critical points still should be tested for local minima
- For convex problems, these conditions are already sufficient conditions for optimality

Example: Solution to the KKT necessary conditions

Arora (2012) Introduction to Optimum Design, Elsevier: Example 4.32 (page 150)

Minimize

$$f(x_1, x_2) = x_1^2 + x_2^2 - 2x_1 - 2x_2 + 2$$

subject to

$$g_1 = -2x_1 - x_2 + 4 \le 0, \ g_2 = -x_1 - 2x_2 + 4 \le 0$$

Objective function and inequality constraints

$$f := (x_1, x_2) \to x_1^2 + x_2^2 - 2 \cdot x_1 - 2 \cdot x_2 + 2 :$$

$$g_1 := (x_1, x_2) \to -2 \cdot x_1 - x_2 + 4 :$$

$$g_2 := (x_1, x_2) \to -x_1 - 2 \cdot x_2 + 4 :$$

Generalized Lagrangian

$$l := f(x_p x_2) + \mu_1 \cdot g_1(x_p x_2) + \mu_2 \cdot g_2(x_p x_2) :$$

$$L := unapply(l, x_1, x_2, \mu_1, \mu_2) :$$

KKT conditions (Stationarity and feasibility)

$$\begin{split} eq_1 &:= \mathsf{D}[\,1\,](\,L)\,\big(\,x_1,\,x_2,\,\mu_1,\,\mu_2\,\big) = 0: \\ eq_2 &:= \mathsf{D}[\,2\,]\,(\,L)\,\big(\,x_1,\,x_2,\,\mu_1,\,\mu_2\,\big) = 0: \\ eq_3 &:= g_1\big(\,x_1,\,x_2\,\big) = G_1: \\ eq_4 &:= g_2\big(\,x_1,\,x_2\,\big) = G_2: \end{split}$$

Equations and unknowns

$$\mathit{eq} := \mathit{unapply} \big(\left\{ \mathit{eq}_1, \mathit{eq}_2, \mathit{eq}_3, \mathit{eq}_4 \right\}, x_1, x_2, \mu_1, \mu_2, G_1, G_2 \big) :$$

KKT conditions (Complementary slackness and dual feasibility)

Check
$$2^n \mu_1, \mu_2, G_1, G_2$$
 combinations for $\mu_1, \mu_2 \ge 0$ and $G_1, G_2 \le 0$

$$case_1 := 0, 0, G_1, G_2 : vars_1 := G_1, G_2 :$$

 $case_2 := 0, \mu_2, G_p, 0 : vars_2 := \mu_2, G_1 :$
 $case_3 := \mu_1, 0, 0, G_2 : vars_3 := \mu_1, G_2 :$

$$\mathit{case}_4 := \mu_1, \mu_2, 0, 0 \colon \mathit{vars}_4 := \mu_1, \mu_2 \colon$$

$$solve(eq(x_{1}, x_{2}, case_{1}), \{x_{1}, x_{2}, vars_{1}\}) = \{G_{1} = 1, G_{2} = 1, x_{1} = 1, x_{2} = 1\}$$

$$solve(eq(x_{1}, x_{2}, case_{2}), \{x_{1}, x_{2}, vars_{2}\}) = \{G_{1} = \frac{1}{5}, \mu_{2} = \frac{2}{5}, x_{1} = \frac{6}{5}, x_{2} = \frac{7}{5}\}$$

$$solve(eq(x_{1}, x_{2}, case_{3}), \{x_{1}, x_{2}, vars_{3}\}) = \{G_{2} = \frac{1}{5}, \mu_{1} = \frac{2}{5}, x_{1} = \frac{7}{5}, x_{2} = \frac{6}{5}\}$$

$$solve(eq(x_{1}, x_{2}, case_{4}), \{x_{1}, x_{2}, vars_{4}\}) = \{\mu_{1} = \frac{2}{9}, \mu_{2} = \frac{2}{9}, x_{1} = \frac{4}{3}, x_{2} = \frac{4}{3}\}$$

Feasible solution: Case 4

$$assign(solve(eq(x_p, x_2, case_4), \{x_p, x_2, vars_4\}))$$

$$x_1, x_2 = \frac{4}{3}, \frac{4}{3}$$

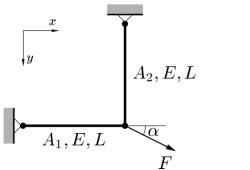
 $\mu_1, \mu_2 = \frac{2}{9}, \frac{2}{9}$

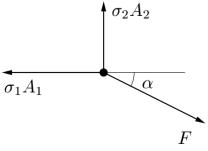
$$f(x_1, x_2) = \frac{2}{9}$$

 $g_1(x_1, x_2), g_2(x_1, x_2) = 0, 0$

Example: Weight minimization with stress constraints

Christensen & Klarbring (2009) An Introduction to Structural Optimization, Springer: Section 2.1 (page 10)





$$\min_{A_1, A_2} A_1 + A_2$$
s.t.
$$\begin{cases}
A_1 \ge \frac{F \cos \alpha}{\sigma_0} \\
A_2 \ge \frac{F \sin \alpha}{\sigma_0}
\end{cases}$$

Objective function and inequality constraints

$$f := (A_{1'}, A_{2}) \rightarrow A_{1} + A_{2}:$$

$$g_{1} := (A_{1'}, A_{2}) \rightarrow \frac{F \cdot \cos(\alpha)}{\sigma \theta} - A_{1}:$$

$$g_{2} := (A_{1'}, A_{2}) \rightarrow \frac{F \cdot \sin(\alpha)}{\sigma \theta} - A_{2}:$$

Generalized Lagrangian

$$\begin{split} I &\coloneqq f \big(A_1, A_2 \big) + \mu_1 \cdot g_1 \big(A_1, A_2 \big) + \mu_2 \cdot g_2 \big(A_1, A_2 \big) : \\ L &\coloneqq unapply \big(I, A_1, A_2, \mu_1, \mu_2 \big) : \end{split}$$

KKT conditions (Stationarity and feasibility)

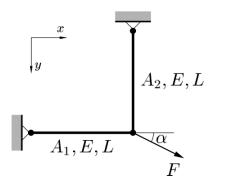
$$\begin{split} eq_1 &:= \ \mathrm{D}[\,1\,](L) \left(A_{l'}A_{2'}\,\mu_{1'}\,\mu_2\right) = 0: \\ eq_2 &:= \ \mathrm{D}[\,2\,](L) \left(A_{l'}A_{2'}\,\mu_{1'}\,\mu_2\right) = 0: \\ eq_3 &:= \ g_1 \Big(A_{l'}A_2\Big) = G_1: \\ eq_4 &:= \ g_2 \Big(A_{l'}A_2\Big) = G_2: \end{split}$$

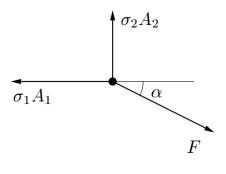
Equations and unknowns

$$\mathit{eq} \coloneqq \mathit{unapply} \left(\left\{ \mathit{eq}_{1'}, \mathit{eq}_{2'}, \mathit{eq}_{3'}, \mathit{eq}_{4} \right\}, A_{1'}, A_{2'}, \mu_{1'}, \mu_{2'}, G_{1}, G_{2} \right) \colon$$

Example: Weight minimization with stress constraints

Christensen & Klarbring (2009) An Introduction to Structural Optimization, Springer: Section 2.1 (page 10)





$$\min_{A_1,A_2} A_1 + A_2$$
s.t.
$$\begin{cases} A_1 \ge \frac{F \cos \alpha}{\sigma_0} \\ A_2 \ge \frac{F \sin \alpha}{\sigma_0} \end{cases}$$

$$A_2^* = \frac{F \sin \alpha}{\sigma_0}$$

KKT conditions (Complementary slackness and dual feasibility)

Check $2^n \mu_1, \mu_2, G_1, G_2$ combinations for $\mu_1, \mu_2 \ge 0$ and $G_1, G_2 \le 0$

$$case_1 := 0, 0, G_1, G_2 : vars_1 := G_1, G_2 :$$

$$case_2 := 0, \mu_2, G_1, 0 : vars_2 := \mu_2, G_1 :$$

$$case_3 := \mu_1, 0, 0, G_2: vars_3 := \mu_1, G_2:$$

$$case_4 := \mu_1, \mu_2, 0, 0 : vars_4 := \mu_1, \mu_2 :$$

$$\begin{split} &eq(A_{1},A_{2},case_{1}) = \left\{1 = 0, \frac{F\cos(\alpha)}{\sigma 0} - A_{1} = G_{1}, \frac{F\sin(\alpha)}{\sigma 0} - A_{2} = G_{2}\right\} \\ &eq(A_{1},A_{2},case_{2}) = \left\{1 = 0, 1 - \mu_{2} = 0, \frac{F\cos(\alpha)}{\sigma 0} - A_{1} = G_{1}, \frac{F\sin(\alpha)}{\sigma 0} - A_{2} = 0\right\} \\ &eq(A_{1},A_{2},case_{3}) = \left\{1 = 0, 1 - \mu_{1} = 0, \frac{F\cos(\alpha)}{\sigma 0} - A_{1} = 0, \frac{F\sin(\alpha)}{\sigma 0} - A_{2} = G_{2}\right\} \\ &eq(A_{1},A_{2},case_{4}) = \left\{1 - \mu_{1} = 0, 1 - \mu_{2} = 0, \frac{F\cos(\alpha)}{\sigma 0} - A_{1} = 0, \frac{F\sin(\alpha)}{\sigma 0} - A_{2} = 0\right\} \end{split}$$

$$solve\big(\textit{eq}\big(A_{\textit{l}}, A_{\textit{2}}, \textit{case}_4\big), \big\{A_{\textit{l}}, A_{\textit{2}}, \textit{vars}_4\big\}\big) = \left\{A_{\textit{l}} = \frac{F\cos\big(\alpha\big)}{\sigma 0}, A_{\textit{2}} = \frac{F\sin\big(\alpha\big)}{\sigma 0}, \mu_{\textit{l}} = 1, \mu_{\textit{2}} = 1\right\}$$

Feasible solution: Case 4

$$assign(solve(eq(A_1, A_2, case_4), \{A_1, A_2, vars_4\}))$$

$$A_{P}A_{2} = \frac{F\cos(\alpha)}{\sigma \theta}, \frac{F\sin(\alpha)}{\sigma \theta}$$

$$\mu_{1}, \mu_{2} = 1, 1$$

$$f(A_1, A_2) = \frac{F\cos(\alpha)}{\sigma \theta} + \frac{F\sin(\alpha)}{\sigma \theta}$$
$$g_1(A_1, A_2), g_2(A_1, A_2) = 0, 0$$

Transforming inequalities into equalities

Arora (2012) Introduction to Optimum Design, Elsevier: Theorem 4.6 (page 142)

Karush-Kuhn-Tucker Optimality Conditions

Let \mathbf{x}^* be a regular point of the feasible set that is a local minimum for $f(\mathbf{x})$, subject to $h_i(\mathbf{x}) = 0$; i = 1 to p; $g_j(\mathbf{x}) \le 0$; j = 1 to m. Then there exist Lagrange multipliers \mathbf{v}^* (a p-vector) and \mathbf{u}^* (an m-vector) such that the Lagrangian function is stationary with respect to x_i , v_i , u_j , and s_j at the point \mathbf{x}^* .

1. Lagrangian Function for the Problem Written in the Standard Form:

$$L(\mathbf{x}, \mathbf{v}, \mathbf{u}, \mathbf{s}) = f(\mathbf{x}) + \sum_{i=1}^{p} v_i h_i(\mathbf{x})$$

$$+ \sum_{j=1}^{m} u_j (g_j(\mathbf{x}) + s_j^2)$$

$$= f(\mathbf{x}) + \mathbf{v}^{\mathsf{T}} \mathbf{h}(\mathbf{x}) + \mathbf{u}^{\mathsf{T}} (\mathbf{g}(\mathbf{x}) + \mathbf{s}^2)$$
(4.46)

2. *Gradient Conditions:*

$$\frac{\partial L}{\partial x_k} = \frac{\partial f}{\partial x_k} + \sum_{i=1}^p v_i^* \frac{\partial h_i}{\partial x_k}$$

$$+ \sum_{i=1}^m u_i^* \frac{\partial g_j}{\partial x_k} = 0; \quad k = 1 \text{ to } n$$
(4.47)

$$\frac{\partial L}{\partial v_i} = 0 \Rightarrow h_i(\mathbf{x}^*) = 0; \quad i = 1 \text{ to } p \tag{4.48}$$

$$\frac{\partial L}{\partial u_j} = 0 \Rightarrow (g_j(\mathbf{x}^*) + s_j^2) = 0; \quad j = 1 \text{ to } m \quad (4.49)$$

3. Feasibility Check for Inequalities:

$$s_j^2 \ge 0$$
; or equivalently $g_j \le 0$;
 $j = 1 \text{ to } m$ (4.50)

4. Switching Conditions:

$$\frac{\partial L}{\partial s_j} = 0 \Rightarrow 2u_j^* s_j = 0; \quad j = 1 \text{ to } m$$
 (4.51)

5. Non-negativity of Lagrange Multipliers for Inequalities:

$$u_i^* \ge 0; \quad j = 1 \text{ to } m$$
 (4.52)

6. Regularity Check: Gradients of the active constraints must be linearly independent. In such a case the Lagrange multipliers for the constraints are unique.

Penalty Methods

- Reformulate a constrained optimization problem as an unconstrained problem
- Penalization of the objective function value when constraints are violated
- Simple example

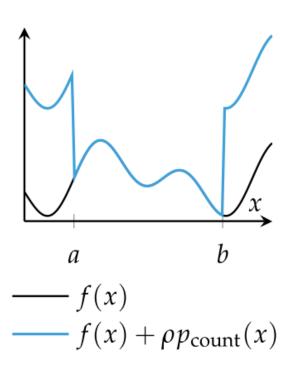
$$\begin{aligned} & \underset{\mathbf{x}}{\text{minimize}} & & f(\mathbf{x}) \\ & \text{subject to} & & \mathbf{g}(\mathbf{x}) \leq \mathbf{0} \\ & & \mathbf{h}(\mathbf{x}) = \mathbf{0} \end{aligned}$$



$$\underset{\mathbf{x}}{\text{minimize}} f(\mathbf{x}) + \rho \cdot p_{\text{count}}(\mathbf{x})$$

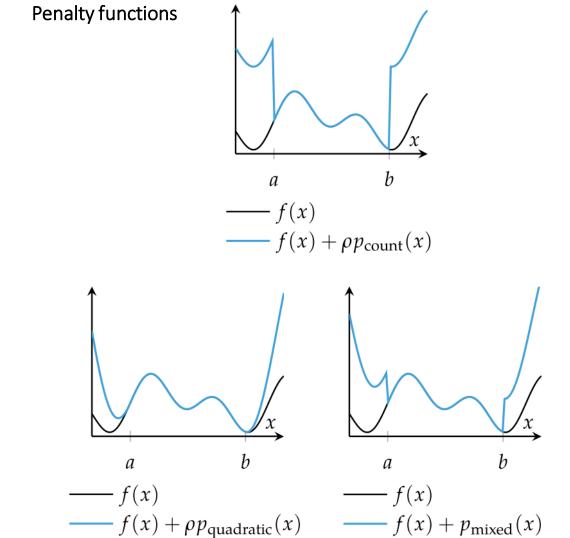
Where ho > 0 adjusts the penalty magnitude

$$p_{\text{count}}(\mathbf{x}) = \sum_{i} (g_i(\mathbf{x}) > 0) + \sum_{j} (h_j(\mathbf{x}) \neq 0)$$



Algorithm for Penalty Methods

- Start with an initial point x and a small value for ρ
- Solve the unconstrained optimization problem
- The resulting design point is then used as the starting point for another optimization with an increased penalty
- We continue with this procedure until the resulting point is feasible or a max number of iterations has been reached



Important notes

$$p_{\text{count}}(\mathbf{x}) = \sum_{i} (g_i(\mathbf{x}) > 0) + \sum_{j} (h_j(\mathbf{x}) \neq 0)$$

 $p_{
m count}$ preserves problem solution for large ho values

- But introduces a sharp discontinuity
- Points not inside the feasible set lack gradient info

$$p_{\text{quadratic}}(\mathbf{x}) = \sum_{i} \max(g_i(\mathbf{x}), 0)^2 + \sum_{j} h_j(\mathbf{x})^2$$

 $p_{
m quadratic}$ very small close to the constrain boundary

• May require ρ to approach infinity before cease violation

$$p_{\text{mixed}}(\mathbf{x}) = \rho_1 p_{\text{count}}(\mathbf{x}) + \rho_2 p_{\text{quadratic}}(\mathbf{x})$$

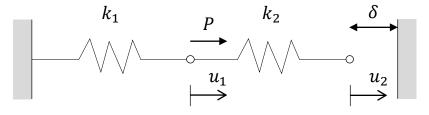
 $p_{
m mixed}$ clear boundary between the feasible/unfeasible regions

Also provides gradient info to the solver

Total Potential Energy

$$\Pi(\boldsymbol{u}) = \frac{1}{2} \boldsymbol{u}^T \boldsymbol{K} \boldsymbol{u} - \boldsymbol{f}^T \boldsymbol{u}$$

Example: Contact Problem



Contact condition

$$u_2 \leq \delta$$

Optimization Problem

minimize
$$\Pi(u_1, u_2) = \frac{1}{2}k_1u_1^2 + \frac{1}{2}k_2(u_2 - u_1)^2 - Pu_1$$

s.t. $u_2 - \delta \le 0$

Contact Problem using Penalty Method

```
In [1]: using Optim, LinearAlgebra
In [2]: # Problem data
         P = 200.
        k_1, k_2, \delta = 1000., 1000., 0.15
        # Stiffness matrix and external force vector
        K = [k_1+k_2 - k_2; -k_2 k_2]
        F = [P, 0.]
        # Total Potential Energy and contact condition
        \Pi(u) = 1/2 * u \cdot (K * u) - (F \cdot u)
        g(u) = u[2] - \delta
        # Penalty function (quadratic)
         p(u) = max(g(u), 0)^2;
In [3]: # minimize: calling Optim unconstained optimize function
        function minimize(f, x0)
             res = optimize(f, x0)
             return Optim.minimizer(res)
In [7]: # Penalty method code
        function penalty_method(f, p, x, k_max; \rho=1, \gamma=2)
             for k in 1 : k max
                 x = minimize(x \rightarrow f(x) + \rho * p(x), x)
                 ρ *= ν
                 if p(x) == 0
                     return x, k, ρ
                 end
                                                            See 04 contactproblem-penalty.ipynb
             return x, k, ρ
In [8]: # Eval contact problem using penalty method
        uopt, k, \rho = penalty_method(\Pi, p, [0., 0], 100)
        println("u*: ", uopt, ", iterations: ", k, ", ρ: ", ρ)
         u* : [0.17500468911768227, 0.14999999945312512], iterations: 46, ρ : 70368744177664
```

Augmented Lagrange Method

Augmented Lagrange Method

- Adaption of penalty method for equality constraints
- Unlike the penalty method, works with smaller values of ρ

$$p_{\text{Lagrange}}(\mathbf{x}) = \frac{1}{2}\rho \sum_{i} (h_i(\mathbf{x}))^2 - \sum_{i} \lambda_i h_i(\mathbf{x})$$

where λ converges towards the Lagrange multiplier

- lacktriangleright
 ho still increases with each iteration
- and also, the linear penalty vector is updated according to

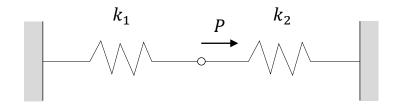
$$\boldsymbol{\lambda}^{(k+1)} = \boldsymbol{\lambda}^{(k)} - \rho \mathbf{h}(\mathbf{x})$$

Algorithm for Augmented Lagrange Method

```
function augmented_lagrange_method(f, h, x, k_max; \rho=1, \gamma=2)
\lambda = zeros(length(h(x)))
for k in 1 : k_max
p = x \rightarrow f(x) + \rho/2*sum(h(x).^2) - \lambda \cdot h(x)
x = minimize(x \rightarrow f(x) + p(x), x)
\rho *= \gamma
\lambda -= \rho*h(x)
end
return x
Julia code for Augmented
Lagrange Method
```

Augmented Lagrange Method

Example: Complementary Energy with Augmented Lagrange Method



Equilibrium condition (internal x external forces)

Complementary Energy

$$\Pi_c(r_1, r_2) = \frac{1}{2} \frac{r_1^2}{k_1} + \frac{1}{2} \frac{r_2^2}{k_2}$$

Optimization Problem

minimize
$$\Pi_c(r_1, r_2)$$

s.t. $r_2 - r_1 = P$

Given this optimization problem

Homework

- Consider:
 - P = 10 kN
 - $k_1 = 100 \text{ kN/m}$
 - $k_2 = 200 \text{ kN/m}$
- Develop an Augmented Lagrange Method routine to solve the problem
 - Consider a break condition if $\Delta \lambda$ is smaller than a given tolerance
- Verify the results with the prementioned analytical solution
- lacktriangle Display the number of iterations and ho value obtained

Interior Point Methods

Interior Point Methods

- Also called Barrier Methods
- Ensure that each step is feasible
- Allows premature termination
 - to return a nearly optimal, feasible point

Barrier Functions, $p_{\text{barrier}}(x)$

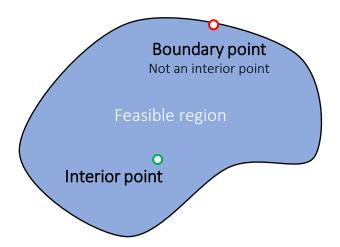
- Similar to penalties but must meet the following conditions:
 - Continuous
 - Non-negative
 - Approach ∞ as \boldsymbol{x} approaches any constraint boundary

Special care with line searches

- Line searches $f(x + \alpha d)$ with $0 < \alpha < \alpha_u$
- α_u is the step to the nearest boundary

Initial guess

Interior Point method requires a feasible point as an initial guess



Interior Point Methods

Examples of barrier functions

Inverse Barrier

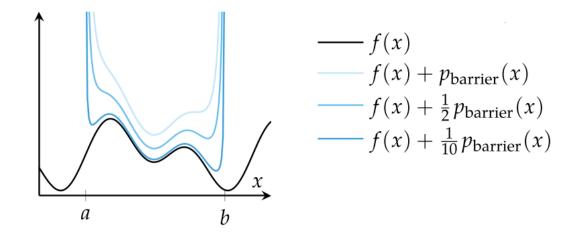
$$p_{\text{barrier}}(\mathbf{x}) = -\sum_{i} \frac{1}{g_i(\mathbf{x})}$$

Log Barrier
$$p_{\text{barrier}}(\mathbf{x}) = -\sum_{i} \begin{cases} \log(-g_i(\mathbf{x})) & \text{if } g_i(\mathbf{x}) \geq -1 \\ 0 & \text{otherwise} \end{cases}$$

A problem with inequality constraints can be transformed into an unconstrained optimization problem

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

Applying interior point method with an inverse barrier for minimizing f s.t. $a \le x \le b$



Questions? Comments?

This presentation and its complementary files

https://github.com/ricardoaf/conopt

New to Julia?

https://github.com/ricardoaf/juliafirststeps

