Solving an optimization problem





Optimisation problem

$$\min_{X_{variable}}$$

$$f(X_{variable}, \pi_{parameters})$$

Objective function

$$h(X_{variable}, \pi_{parameters}) = 0$$

m : Model

n : Decision Variables

$$X_{variable} - \pi_{specification} = 0$$

Specifications

$$g(X_{variable}) \le 0$$

Constraints

$$X_{variable,min} \leq X_{variable} \leq X_{variable,max}$$

Degrees of freedom: n-m

Solving method

The goal of the optimisation is to fix the value of the n-m degrees of freedom

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Non linear Optimisation methods: iterative

Direct search

- -Exploring the search space from a location to find the lowest point
 - Easy to use and robust
 - High computing time

Indirect search

- -Mathematical condition of the optimality
 - More efficient
 - More complex (derivatives)

Heuristic methods

- -Explore the search space based on a property of the system
 - e.g. genetic algorithms
 - Global optimum
 - Very high computing time
 - Highly dependent on the quality of the model





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Direct search methods

Unconstrained problems Black Box Approach

$$\min_{X_{decision}} f(X_{decision})$$

 $X_{decision,min} \le X_{decision} \le X_{decision,max}$





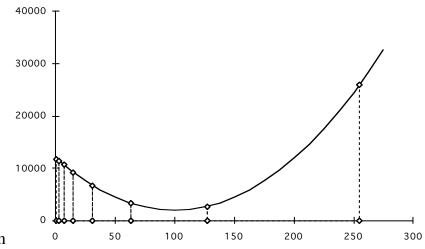
I DOF method

From the best points : generate a new point and eliminate the worst one

Direct search

Interval reduction

$$x_{\min} < x_1 < x_2 < x_{\max}$$



-Gold number
$$x_{\text{max}} - x_2 = x_1 - x_{\text{min}}$$

$$et \frac{x_1 - x_{\text{min}}}{x_{\text{max}} - x_1} = \frac{x_{\text{max}} - x_1}{x_{\text{max}} - x_{\text{min}}} = \frac{\sqrt{5} - 1}{2} \approx 0,618$$

Polynomial approximation

$$f(x) = a + bx + cx^2 \Rightarrow \frac{\delta f}{\delta x} \Big]^* = 0 \Rightarrow x^* = \frac{-b}{2c}$$

With 3 points

$$x^* = \frac{1}{2} \frac{\left(x_2^2 - x_3^2\right) \cdot f_1 + \left(x_3^2 - x_1^2\right) \cdot f_2 + \left(x_1^2 - x_2^2\right) \cdot f_3}{\left(x_2 - x_3\right) \cdot f_1 + \left(x_3 - x_1\right) \cdot f_2 + \left(x_1 - x_2\right) \cdot f_3}$$



Unconstrainted, multi variables

- Irst order, follow the slope
 - + choose the distance (I dimension problem)

distance direction
$$x^{k+1} = x^k + \lambda^k s^k = x^k - \lambda^k \nabla f(x^k)$$
Slope calculation

Linear approximation from previous steps Numerical calculation of derivatives

distance : λ^k

fixed size

► I dimension optimisation

$$\min_{\lambda^k} f(x^{k+1})$$





Indirect search methods

- Unconstrained problem
- Express the conditions of optimality

$$\min_{X_{decision}} f(X_{decision})$$
is equivalent to
$$\nabla f(X_{decision}) = 0$$

- Transform optimisation into solving a set of equations
 - -N variables => N derivatives => NxN problem (0 DOF)
- Inequalities = safe guards => constrained problems

$$X_{decision,min} \le X_{decision} \le X_{decision,max}$$





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2nd order method: quadratic approximation

Newton method

$$f(x) \approx q(x) = f(x^k) + \nabla^T f(x^k) \Delta x^k + \frac{1}{2} (\Delta x^k)^T H(x^k) (\Delta x^k)$$

$$\nabla q(x) = 0 \Rightarrow \nabla f(x^k) + H(x^k) (\Delta x^k) = 0$$

$$x^{k+1} - x^k = \Delta x^k = -[H(x^k)]^{-1} \nabla f(x^k)$$
with $H(x^k) = \frac{\delta^2 f(x)}{\delta x_i \delta x_j}$ Hessian Matrix 2nd derivative!

when H is not definite positive \Rightarrow H = H + β I

$$\beta >>$$
 steepest descent

$$\beta << Newton$$

$$\nabla f(x^k) = \frac{\delta f(x)}{\delta x_i} : gradient$$





Indirect search methods

Constrained problems

Simultaneous approach Two level approach

$$\min_{X_{decision}}$$

$$f(X_{decision})$$

$$h(X_{decision}) = 0$$

$$g(X_{decision}) \le 0$$

$$X_{decision,min} \leq X_{decision} \leq X_{decision,max}$$





Constrained programming

• Canonical formulation:

$$min f(\underline{x})$$

Subject to
$$h_j(\underline{x}) = 0$$
 $j=1,...,n_h$ $g_k(\underline{x}) \ge 0$ $k=1,...,n_g$

Inequality constraints are first converted into equalities by adding 1 equation and 1 variable ($s_k \ge 0$): The slag variable

$$g_k(\underline{x}) - s_k^2 = 0$$
 $k=1,...,n_g$

New problem

min
$$f(\underline{x})$$
 $\underline{x}=[x_1,x_2,...,x_n, s_g]$

Subject to $h_j(\underline{x}) = 0$ $j=1,...,n_h$

$$g_{k}(\underline{x}) - s_{k}^{2} = 0 \quad k=1,...,n_{g}$$

 $X_{v,min} \le X_v \le X_{v,max} v = 1,...,n_v$

$$s_k \ge 0$$
 $k=1,...,n_g$





Constrained programming

New problem

$$\min f(\underline{x})$$

$$\underline{\times} = [\times | , \times 2, \dots, \times_n, s_g]$$

Subject to

$$h_i(\underline{x}) = 0$$

$$h_{j}(\underline{x}) = 0$$
 $j=1,...,n_{h}$

$$g_{k}(\underline{x}) - s_{k}^{2} = 0 \quad k=1,...,n_{g}$$

$$X_{v,min} \le X_v \le X_{v,max} v=1,...,n_V$$

$$s_k \ge 0$$
 $k=1,...,n_g$



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Reduced gradient

- Variables are divided into two groups :
 - **Basic** Variables are calculated by solving the set of equations for fixed values of the **Non Basic** variables

$$X_{base} = X(X_{nbase}) : h(X_{base}, X_{nbase}) = 0$$

solve

$$h(X_{base}, \chi_{nbase}) = 0$$

$$\chi_{nbase} - X_{Nbase} = 0$$

For given values of X_{Nbase}

New unconstrained problem

$$min_{X_{nbase}} F(X(X_{nbase}), X_{nbase})$$

subject to $X_{min} \leq X_{base}(X_{nbase}) \leq X_{max}$

$$S(X_{nbase})? \geq 0$$
 !!! non linear inequality





Generalised Reduced Gradient (GRG)

- Variables are divided into two groups: Basic and Non Basic variables
- Use slack variables for inequalities
- Search by conjugate direction => unconstrained problem within bounds
 - —Optimisation search is realised in the nbase domain, the basic variables are calculated by solving:

$$h(x_{base}, x_{nbase}) = 0 \Rightarrow \frac{\partial h}{\partial x} = \left(\frac{\partial h}{\partial x_{base}}, \frac{\partial h}{\partial x_{nbase}}\right) = \left(B_{base}, B_{nbase}\right)$$

With
$$\frac{\partial h}{\partial x_{base}} : n_h \times n_h \Rightarrow x_{base} = \varphi(x_{nbase})$$

and $f(x_{base}, x_{nbase})$ becomes $F(x_{base}(x_{nbase}), x_{nbase})$

$$F(x_{base}(x_{nbase}), x_{nbase})$$

Reduced Gradient
$$\frac{\partial F}{\partial x_{nbase}} = \frac{\partial f}{\partial x_{nbase}} - z^T B_{nbase}$$

Where
$$z^T = (B_{base})^{-1} \frac{\partial f}{\partial x_{base}}$$



Constrained programming: Lagrange equivalence

Problem equivalence

Original : decision variable : n_V + n_g

$$\min_{\mathbf{X}} f(\underline{\mathbf{x}}) \qquad \underline{\mathbf{x}} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_V], \ \underline{\mathbf{s}} = [\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_g]$$
 Submitted to
$$h_j(\underline{\mathbf{x}}) = 0 \qquad \qquad j = 1, \dots, n_h$$

$$g_k(\underline{\mathbf{x}}) \cdot \underline{\mathbf{s}}_k^2 = 0 \qquad \qquad k = 1, \dots, n_g$$

Lagrange equivalent : decision variables : n_V + n_h + 2 n_g

min
$$L(x,\lambda) = f(x) + \sum_{j=1}^{n_h} \lambda_j h_j(x) + \sum_{k=1}^{n_g} \mu_k [g_k(x) - s_k^2]$$

decision variables $x_{v,min} \le x_v \le x_{v,max}$ $v=1,...,n_v$

 n_g slag variables $s_k \ge 0$ $k=1,...,n_g$

 $\begin{array}{lll} & & & & \\ & & \\ n_h + n_g \text{ new variables}: & & \lambda_j \leq 0 & & j=1,\dots,n_h \\ & & & \\ Langrangian \text{ multipliers} & & \mu_k \leq 0 & & k=1,\dots,n_g \end{array}$



Lagrange formulation

 the goal is to transform a constrained problem into a non constrained problem but with a higher problem size :

$$L(x,\lambda) = f(x) + \sum_{j=1}^{n_h} \lambda_j h_j(x) + \sum_{k=1}^{n_g} \mu_k [g_k(x) - s_k^2]$$

-to be minimised with respect to x, s and λ , μ

- There are therefore (nx+ nh +2 ng variables)
- Necessary optimality conditions

$$\lambda_{j} \leq 0 \quad j = 1, ..., n_{h}$$

$$\mu_{k} \leq 0 \quad k = 1, ..., n_{g}$$

$$\frac{\delta L(x^*, s^*, \lambda^*, \mu^*)}{\delta x_i} = 0 i = 1, ..., n_x$$

$$\frac{\delta L(x^*, s^*, \lambda^*, \mu^*)}{\delta s_g} = 0 g = 1, ..., n_g$$

$$\frac{\delta L(x^*, s^*, \lambda^*, \mu^*)}{\delta \lambda_h} = 0 h = 1, ..., n_h$$

$$\frac{\delta L(x^*, s^*, \lambda^*, \mu^*)}{\delta \mu_g} = 0 g = 1, ..., n_g$$





$$\nabla_{x,s,\lambda,\mu} L(x,s,\lambda,\mu) = 0$$

$$\lambda_j \le 0 \quad j = 1,...,n_h$$

$$\mu_k \le 0 \quad k = 1,...,n_g$$

Square system: $n_x + n_h + 2 n_g$

$$\frac{\partial L(x^*)}{\partial x_i} = \frac{\partial f(x^*)}{\partial x_i} + \sum_{j=1}^{n_h} \lambda_j \frac{\partial h_j(x^*)}{\partial x_i} + \sum_{k=1}^{n_g} \mu_k \left[\frac{\partial g_k(x^*)}{\partial x_i}\right] = 0 \qquad i = 1, ..., n_x$$

$$\frac{\partial L(x^*)}{\partial \lambda_j} = h_j(x) = 0 \qquad j = 1, ..., n_h$$

$$\frac{\partial L(x^*)}{\partial \mu_k} = g_k(x) - s_k^2 = 0 \qquad k = 1, ..., n_g$$

$$\frac{\partial L(x^*)}{\partial s_k} = 2 \ \mu_k \ s_k = 0 \quad k = 1, ..., n_g$$

We calculate the variables, the slags and the Lagrange multipliers at the same time!

<- Difficult to solve

Explanation λ_i

$$\lambda_{j}^{*} = \frac{\delta f^{*}}{\delta h_{j}} \quad \mu_{k}^{*} = \frac{\delta f^{*}}{\delta g_{k}}$$

- What is the penalty of a constraint?
- -Without the constraint the objective function is better, the multipliers measures of how much
- -Important for inequality constraints

Example:

Minimise the time for transporting goods with a maximum of 3 trucks Constraint: maximum 3 trucks

 λ = what is the time benefit when adding I truck



Solving the equations step by Newton step

at iteration r

$$\nabla L \approx \nabla L^r + \mathbb{H}^r \Delta x_i^{r+1} = 0$$

$$\frac{\partial f(x^*)}{\partial x_i} + \sum_{j=1}^{n_h} \lambda_j \frac{\partial h_j(x^*)}{\partial x_i} + \sum_{k=1}^{n_g} \mu_k \left[\frac{\partial g_k(x^*)}{\partial x_i} \right] = 0$$

$$h_j(x) = 0$$

$$g_k(x) - s_k^2 = 0$$

$$2 \mu_k s_k = 0$$

$$\frac{\partial f(x^{*})}{\partial x_{i}} + \sum_{j=1}^{n_{h}} \lambda_{j} \frac{\partial h_{j}(x^{*})}{\partial x_{i}} + \sum_{k=1}^{n_{g}} \mu_{k} \left[\frac{\partial g_{k}(x^{*})}{\partial x_{i}} \right] = 0$$

$$h_{j}(x) = 0$$

$$g_{k}(x) - s_{k}^{2} = 0$$

$$2 \mu_{k} s_{k} = 0$$

$$\frac{\partial f(x^{*})}{\partial x_{i}} + \sum_{k=1}^{n_{g}} \mu_{k} \left[\frac{\partial g_{k}(x^{*})}{\partial x_{i}} \right] = 0$$

$$B^{r} \quad 0 \quad 0 \quad 0$$

$$B^{r} \quad 0 \quad 0 \quad -2Is^{r}$$

$$0 \quad 0 \quad Is^{r} \quad I\mu^{r}$$

$$\Delta x^{r+1}$$

$$\Delta x^{r+1}$$

$$\Delta x^{r+1}$$

with

$$H^{r} = \frac{\partial^{2} f(x^{r})}{\partial x_{i} \partial x_{j}} \Big]^{r} + \sum_{j=1}^{n_{h}} \lambda_{j} \frac{\partial^{2} h_{j}(x^{r})}{\partial x_{i} \partial x_{j}} \Big]^{r} + \sum_{k=1}^{n_{g}} \mu_{k} \frac{\partial^{2} g_{k}(x^{r})}{\partial x_{i} \partial x_{j}} \Big]^{r}$$

$$A^{r} = \frac{\partial f(x^{r})}{\partial x_{i}}, B^{r} = \frac{\partial g(x^{r})}{\partial x_{i}}$$



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Solving the equations set by Newton step

$$\nabla L \approx \nabla L^r + \mathbb{H}^r \Delta x_i^{r+1} = 0$$

$$\Delta x_i^{r+1} = -\mathbb{H}^{r-1} \nabla L^r$$

$$x_i^{r+1} = x_i^r + (1 - q)\Delta x_i^{r+1}$$

Note: for linear problems

 \mathbb{H}^r is constant q=0 (no relaxation)

Problem : find which s or μ = 0

$$\begin{bmatrix} H^r & A^r & B^r & 0 \\ A^{r^T} & 0 & 0 & 0 \\ B^{r^T} & 0 & 0 & -2Is^r \\ 0 & 0 & Is^r & I\mu^r \end{bmatrix} \begin{bmatrix} \Delta X^{r+1} \\ \Delta \lambda^{r+1} \\ \Delta \mu^{r+1} \\ \Delta s^{r+1} \end{bmatrix} = \nabla L^r$$

with

$$H^{r} = \frac{\partial^{2} f(x^{r})}{\partial x_{i} \partial x_{j}} \bigg]^{r} + \sum_{j=1}^{n_{h}} \lambda_{j} \frac{\partial^{2} h_{j}(x^{r})}{\partial x_{i} \partial x_{j}} \bigg]^{r} + \sum_{k=1}^{n_{g}} \mu_{k} \frac{\partial^{2} g_{k}(x^{r})}{\partial x_{i} \partial x_{j}} \bigg]^{r}$$

$$A^{r} = \frac{\partial f(x^{r})}{\partial x_{i}}, B^{r} = \frac{\partial g(x^{r})}{\partial x_{i}}$$



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Successive Quadratic Programming

- Quadratic approximation of the Langrangian
 - -Quadratic Approximation of the objective function

$$\left[\nabla f(x^0)\right]^T \Delta x + (\Delta x)^T Q \Delta x$$

Q is the quadratic approximation of

$$\nabla^2 L = \nabla^2 (f - \lambda^T h - \mu^T g)$$

or other method to update Q

- Linearised constraints
- -Defines
 - -the direction
 - -step lenght
- -Penality when the points is infeasible
- Iterative procedure



Mixed Integer Problems

MILP

- -Mixed Integer Linear Programming problems
 - Linear constraints & objective
 - continuous and integer variables

MINLP

- Mixed Integer Non Linear Programming problems
 - Non linear constraints & objective
 - continuous and integer variables





MINLP: outer approximation

Decomposition theorem

- -Partition variables in 2 sets
 - complicating set (integer)
 - continuous variables
- -Solve 2 problems
 - NLP with fixed integer (lower bound)
 - MILP: outer-approximate the objective function (upper bound)
- -Lower = upper => convergence
 - integer cut to avoid looping

• Problems:

- -NLP converge?
- Calculation time ?
- Initial set feasible ?
- -Derivatives for MILP
 - outer approximation

