Tutorial

Nonlinear Optimization

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Motivation : Nonlinear Optimization in Statistics (I)

*"**All statistical procedures are, in the ultimate analysis, solutions to suitably formulated optimization problems**. Whether it is designing a scientific experiment, or planning a large-scale survey for collection of data, or choosing a stochastic model to characterize observed data, or drawing inference from available data, such as estimation, testing of hypotheses, and decision making, **one has to choose an objective function and minimize or maximize it subject to given constraints on unknown parameters and inputs** such as the costs involved."*

C.R. Rao, in "*Mathematical Programming in Statistics*", Arthanary and Dodge 1993

Motivation : Nonlinear Optimization in Statistics (II)

- This tutorial will be restricted to **Nonlinear Optimization** techniques, useful for:
  - Maximization of a likelihood function.
  - Nonlinear regression.
  - ...
- We will not cover other optimization techniques as:
  - Combinatorial optimization.
  - Global optimization.
  - Nondifferentiable optimization.
  - Heuristics.
- Let's go now to the contents of this tutorial... ▶

Maximization of the likelihood function

- **Current status Covariates in a simple linear model (Langohr, Gómez)**
  - **Model :** $Y = \alpha + \beta Z + \varepsilon \quad ; \quad Y \in \Re^n, Z \in \Re, \varepsilon \in \Re^n$

    $\varepsilon \sim N(0, \sigma^2 I_n) \Rightarrow Y \mid Z \sim N(\alpha + \beta Z, \sigma^2 I_n)$

    Decision variables è $= [\alpha \quad \beta \quad \sigma]^T \in \Re^3$, $\sigma \geq 0$ **Constraints**
  - Z is the ***Current Status Covariate*** with cumulative distribution $W(z)$: the only observation is whether Z exceeds the observed value z_i or not; δ_i is the corresponding indicator variable: $\delta_i = 1_{\{Z \leq z_i\}}$
  - **Observations :** $[y_i \quad z_i \quad \delta_i], i = 1, 2, \ldots, n$
  - **Covariate :** Z is supposed to be discrete with possible (ordered) values $s_1, s_2, \ldots, s_m$ and corresponding probabilities $\omega_j = P(Z = s_j)$, $j = 1, \ldots, m$:

    Decision variables ù $= [\omega_1, \ldots, \omega_m]^T$, **Constraints** $\omega_j \geq 0$, $\sum_{j=1}^{m} \omega_j = 1$

Maximization of the likelihood function

- **Maximum likelihood function :**

$$L_n(\text{ù},\text{è}) = \prod_{i=1}^{n}\sum_{j=1}^{m}\gamma_{ij} f(y_i \mid s_j;\text{è})\omega_j =$$

Objective function $f(x)$

$$= \prod_{i=1}^{n}\sum_{j=1}^{m}\gamma_{ij}\frac{1}{\sigma\sqrt{2\pi}}\left(e^{-\frac{1}{2}\frac{(y_i-\alpha-\beta s_j)^2}{\sigma^2}}\right)\omega_j$$

$$\gamma_{ij} = 1_{\{s_j \in I_i\}} \quad , \quad I_i = \begin{cases} [s_1 , z_i] & \text{if } \delta_i = 1 \\ (z_i , s_m] & \text{otherwise} \end{cases}$$

- The problem above corresponds to a *Linearly Constrained Nonlinear Optimization Problem* (LCNOP):

(LCNOP) $\max_x \{ f(x) \mid x \in X \}$; $X = \{ x \in \Re^n \mid Ax = b, l \leq x \leq u \}$

Nonlinear regression: SIDS

- **Sudden Infant Death Syndrome:**
  - The following nonlinear model was considered by Murphy and Campbell (1987) as a part of their study of the Sudden Infant Death Syndrome (SIDS).
  - Given a data series of the daily temperature t_{ij} in day j of year i (j=1,2,...,365 , i=1,2,...,5), the authors proposed the following harmonic model:

$$t_{ij}(a_i, b_i, c_i) = a_i \cos\left(\frac{2\pi}{365} j - b_i\right) + c_i$$

Decision variables x

$$i = 1,2,3,4,5$$

$$j = 1,2,\ldots,365$$

Nonlinear regression: SIDS

- **Nonlinear optimization problem associated to the SIDS model:**

Objective function $f(x)$

$$\min_{\substack{a_i, b_i, c_i \\ i=1,2,\ldots,5}} \frac{1}{2}\sum_{i=1}^{5}\sum_{j=1}^{365}\left[t_{ij}(a_i, b_i, c_i) - t_{ij}\right]^2$$

(Nonlinear Least-Squares Problem)

- The problem above corresponds to an ***Unconstrained Nonlinear Optimization Problem (UNOP)*** :

(UNOP) $\min_{x \in \Re^n} f(x)$

- If *smoothness conditions* are added to the model, the problem becomes a ***Generally Constrained NOP*** :

(GCNOP) $\min_x \{ f(x) \mid x \in X \}$; $X = \{ x \in \Re^n \mid h(x) = 0,\ g(x) \leq 0 \}$

Summary

Nonlinear Optimization Problem (NOP)

- The general (standard) form of the NOP is :

$$(\text{NOP})\begin{cases}\min\limits_{x\in\Re^n} & f(x) & \textbf{Objective function}\\ \text{subject to:} & h(x)=0 & \textbf{Equality constraints}\\ & g(x)\le 0 & \textbf{Inequality constraints}\end{cases}$$

where $x\in\Re^n$ are the **decision variables**, or simply, **variables**, and

$$f:\Re^n\to\Re \qquad h:\Re^n\to\Re^m \qquad g:\Re^n\to\Re^l$$

- Usually, f, h and g are required to be differentiable and "smooth" (*Lipschitz continuous*, or so) to guarantee good properties of the algorithms.
- Of course, $\max f(x) \equiv \min -f(x)$

Classification of the NOP accordingly with the solution

- Consider the NOP expressed in the following way:

$$(\text{NOP})\ \min_x\{f(x)\mid x\in X\}\ ;\ X=\{x\in\Re^n \mid h(x)=0,\ g(x)\le 0\}$$

(X is known as the **feasible set**)

- **NOP with optimal solution:** The set $\{f(x)|x\in X\}$ is bounded below
  $$\min_x\{f(x)=x_1^2+x_2^2 \mid x\ge 0\}$$
- **Infeasible problem** : the feasible set X is empty:
  $$\min_x\{f(x)=x_1^2+x_2^2 \mid x_1+x_2\le -1,\ x\ge 0\}$$
- **Unbounded problem:** The set $\{f(x)|x\in X\}$ is unbounded below
  $$\min_x\{f(x)=-x_1^2-x_2^2 \mid x\ge 0\}$$
- **Existence of at least one global minimum**: guaranteed if f is continuous and $X\subseteq\Re^n$ compact (*Weierstrass Theorem*)

Classification of the NOP accordingly with the formulation

- **Unconstrained NOP:**
  $$(\text{UNOP})\ \min_{x\in\Re^n} f(x)$$
- **NOP with Simple Bounds:**
  $$(\text{SBNOP})\ \min_x\{f(x)|l\le x\le u\}$$
- **Linearly Constrained NOP:**
  $$(\text{LCNOP})\ \min_x\{f(x)|x\in X\}\ ;\ X=\{x\in\Re^n|Ax=b, l\le x\le u\}$$
- **Generally Constrained NOP:**
  $$(\text{GCNOP})\ \min_x\{f(x)\mid x\in X\}\ ;\ X=\{x\in\Re^n \mid h(x)=0,\ g(x)\le 0\}$$

General strategy of the NO algorithms

- Given the feasible bounded NOP:

$$(\text{NOP})\ \min_x\{f(x)\mid x\in X\}\ ;\ X=\{x\in\Re^n \mid h(x)=0,\ g(x)\le 0\}$$

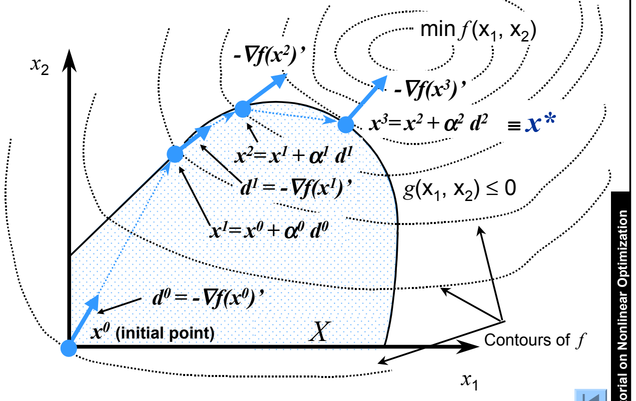
the general strategy followed by most of the NO alg. is:

1. Find a first feasible solution $x\in X$ (current solution).

2. If the current solution x satisfies the optimality conditions, then STOP: $x^*:=x$

3. If the current solution x does not satisfies the optimality conditions, find, using the local information available on x, a new feasible iterate $x\in X$ that improves the value of some merit function related with the objective function $f(x)$, or the objective function itself. Go to 2 with the new current iterate.

General strategy of the NO algorithms

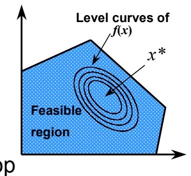


Desirable properties of the NO algorithms

- **Robustness**: they should perform well...
  - … on a wide variety of problems in their class
  - … for all reasonable choices of the initial variables
  - …without the need of "tuning".
- **Efficiency**: low execution time and memory requirements
- **Accuracy**: they should be able to identify the solution with precision without being affected by errors in the data or arithmetic rounding errors.

Local and Global optimization

- The methods presented here only seek for **local optima**
  - They converge to a point satisfying the first order optimality conditions (or second order, depending on the algorithm).
- **Convexity** : any local optima is global if the NOP is **convex**, that is:
  - If the objective function $f(x)$ is convex.
  - If the feasible set X is convex.
  - Example: minimization of a quadratic pos. def $f(x)$ over a politop



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- NAG Numerical Libraries: www.nag.co.uk/numeric/numerical_libraries.asp
- PROC NLP (SAS Optimization Software) www-fp.mcs.anl.gov/otc/Guide/SoftwareGuide/Blurbs/procnlp.html

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Tutorial on Nonlinear Optimization

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Algorithms for Unconstrained Nonlinear Optimization

Unconstrained Nonlinear Optimization

- **Fundamentals**
  - General framework: optimality conditions; descent directions; linesearch
  - Measures of performance of the algorithms: global convergence; local convergence.
- **Methods that use first derivatives**
  - Steepest Descent method (SD)
  - Conjugate Gradient method (CG)
  - Quasi-Newton method (QN)
- **Methods that use second derivatives**
  - Newton and Modified Newton methods (N, MN)
- **Nonderivative methods**
  - Finite differences, coordinate descent and direct search.
- **Nonlinear Least-squares problems**:
  - Gauss-Newton method (GN).

Fundamentals:
General Framework

Given (UNOP) $\min_{x\in\Re^n} f(x)$ **, generate a sequence** $\{x^k\}_{k=0}^{\infty}$ **that converges to the optimal solution** x^*

1. Initialize $x^k \in X \equiv \Re^n$ (current solution). $k:=0$

2. If the current solution x^k satisfies the **stopping criterium**, then $x^* := x^k$. **STOP**:

3. If x^k is not the optimal solution, find a new iterate that improves enough the value of the objective function, and take it as the new iterate. This is performed through the following steps:

- **3.1.** Computation of a **descent direction** d^k
- **3.2.** Computation of a **steplength** α^k
- **3.3.** Update: $x^{k+1} := x^k + \alpha^k d^k$, $k:=k+1$. Go to 2

Fundamentals:
Stopping criterium: optimality conditions

- **First-Order Necessary Conditions** — **Usual stopping criterium**

  "If x^* is a local minimizer and f is continuously differentiable in an open neighbourhood of x^*, then $\nabla f(x^*)=0$"

- **Second-Order Necessary Conditions**

  *"If x^* is a local minimizer and f and $\nabla^2 f$ is continuous in an open neighbourhood of x^*, then $\nabla f(x^*)=0$ and $\nabla^2 f(x^*)$ is **positive semidefinite**"*

- **Second-Order Sufficient Conditions.**

  *"Suppose that $\nabla^2 f$ is continuous in an open neighbourhood of x^* and that $\nabla f(x^*)=0$ and $\nabla^2 f(x^*)$ is **positive definite**. Then x^* is a **strict** local minimizer and f"*

- **The role of convexity.**

  *"When **f is convex**, any local minimizer x^* is a global minimizer of f. If, in addition, f is **differentiable**, then **any stationary point x^* is a global minimizer of f**"*

Fundamentals:

Practical stopping criterium

- The robust numerical implementation of the stopping criterium $\|\nabla f(x^k)\|\approx \mathbf{0}$ could be quite sophisticated. The algorithm will stop either ...

  ... If the measure of the relative size of the gradient at x^k is small:

$$\max_{1\le i\le n}\left|\frac{\max\{|x_i^k|,1\}}{\max\{|f(x^k)|,1\}}\nabla f(x^k)_i\right|\le \varepsilon^{\frac{1}{3}}$$

  ... or the measure of the relative change of the variables x^k in the last step is small :

$$\max_{1\le i\le n}\left|\frac{|x_i^{k+1}-x_i^k|}{\max\{x_i^k,1\}}\right|\le \varepsilon^{\frac{2}{3}}$$

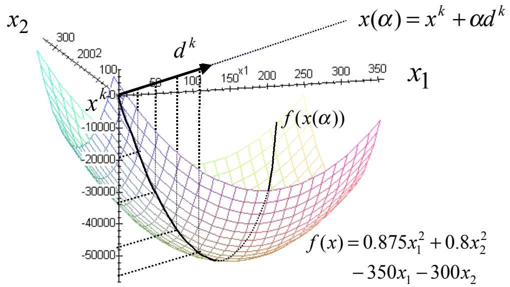
Where ε is the machine precision

Fundamentals:

Descent directions : definition

- **Descent direction :**

  $d^k\in\Re^n$ is a descent direction for the problem UNOP over x^k if: $\exists\,\overline{\alpha}\in\Re^+\ \big|\ \forall\alpha\in[0,\overline{\alpha}]:\ f(x^k+\alpha d^k)<f(x^k)$

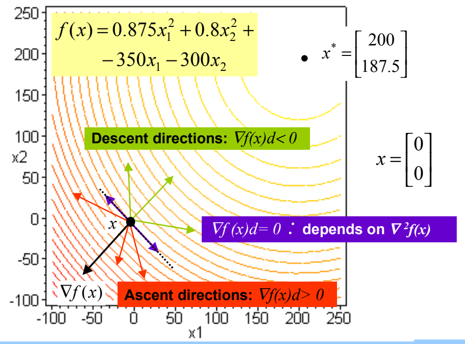


Fundamentals:

Descent directions : identification

- **Sufficient condition of descent:**

  If $\nabla f(x)d<0$ then d is a descent direction for $f(x)$ at x.



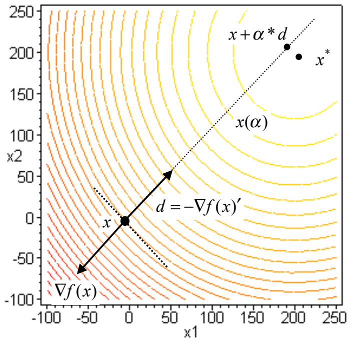
Fundamentals:

Descent directions : computation

- **Methods that use firsts derivatives:**
  - **Steepest descent:** $d^k=-\nabla f(x^k)$
  - **Conjugate Gradient:** $d^k=-\nabla f(x^k)+\beta^k d^{k-1}$
  - **Quasi-Newton Methods:** $d^k=-B^k\nabla f(x^k)$, B^k simetric, pos. def.
- **Methods that use second derivatives:**
  - **Newton Method :** $d^k=-[\nabla^2 f(x^k)]^{-1}\nabla f(x^k)$
- The properties of these methods will be studied later.

Fundamentals:

Steplength



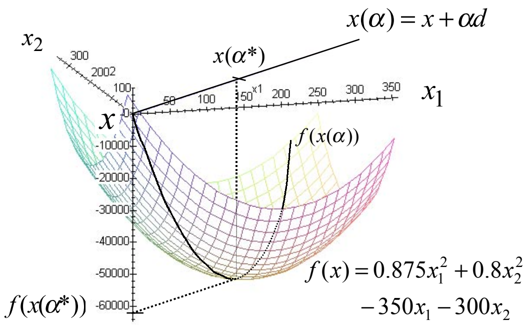
- x is the current iterate
- d is the current search descent direction (for instance $d=-\nabla f(x)'$)
- The next iterate will lie in the half line $x(\alpha)= x+\alpha d$, $\alpha \geq 0$
- We must decide how far to move from x along d:

steplength α^*

Fundamentals:

Computing the steplength: linesearch

- **Linesearch** : $\alpha^*=\text{argmin}\{ f(x+\alpha d) \mid \alpha \geq 0 \}$



Fundamentals:

Exact linesearch (quadratic functions)

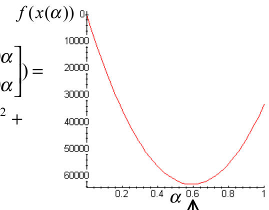
- **Linesearch** : $\alpha^*=\text{argmin}\{ f(x+\alpha d) \mid \alpha \geq 0 \}$
- In our example: $\min_{x\in\Re^n} f(x)=0.875x_1^2+0.8x_2^2-350x_1-300x_2$

$$x=\begin{bmatrix}0\\0\end{bmatrix} \; ; \; d=-\nabla f(x)'=\begin{bmatrix}350\\300\end{bmatrix} \quad \left(\nabla f(x)d=-\|\nabla f(x)\|<0\right)$$

$$f(x(\alpha))=f(x+\alpha d)=$$

$$=f\left(\begin{bmatrix}0\\0\end{bmatrix}+\alpha\begin{bmatrix}350\\300\end{bmatrix}\right)=f\left(\begin{bmatrix}350\alpha\\300\alpha\end{bmatrix}\right)=$$

$$=0.875(350\alpha)^2+0.8(300\alpha)^2+$$
$$-350(350\alpha)-300(300\alpha)$$
$$=179187.5\alpha^2-212500\alpha$$



$$\frac{df(x(\alpha^*))}{d\alpha}=358375\alpha^*-212500=0 \; ; \; \alpha^*=0.5939$$

Fundamentals:

Inexact linesearch (general functions)

- **Problem:** when $f(x)$ is not quadratic the optimal steplength α^* must be estimated numerically.
- **Purpose of the inexact linesearch** :
  to identify $\alpha^k \approx \text{argmin}\{ f(x^k+\alpha^k d^k) \mid \alpha \geq 0 \}$ such that...
  … provides significant reduction of $f(x)$
  … without spending too much time in the computation.
- **Rationale of the inexact linesearch methods**:
  - Define a criterium for the *sufficient decrease* in $f(x)$
  - Find somehow an interval [α_{min} , α_{max}] containing α^*.
  - Set $\alpha := \alpha_{max}$, the trial steplength.
  - Repeat Until $f(x^k+\alpha d^k)$ satisfies the ***sufficient decrease condition***
    Find (bisection, interpolation) a trial steplength $\alpha \in$ [α_{min} , α_{max}]
    Update [α_{min} , α_{max}] .
    End Repeat
  - Set $\alpha^k := \alpha$.

Fundamentals:

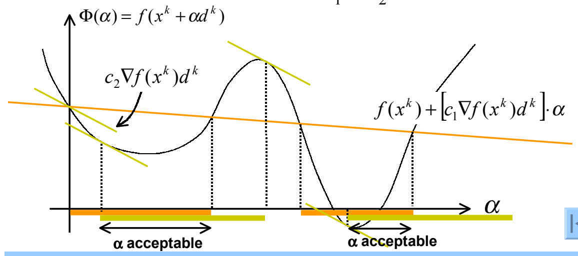
Inexact linesearch (general functions)

- **Sufficient decrease condition:** (Wolfe conditions)

$$f(x^k+\alpha d^k) \le f(x^k) + [c_1 \nabla f(x^k) d^k]\cdot\alpha \quad \text{(W1)}$$

$$\nabla f(x^k+\alpha d^k) d^k \ge c_2 \nabla f(x^k) d^k \quad \text{(W2)}$$

$$0 < c_1 < c_2 < 1$$



Fundamentals:

Measures of performance of an algorithm

- Global convergence: an algorithm is said to be "globally convergent" if

$$\lim_{k\to\infty} \left\| \nabla f(x^k) \right\| = 0$$

  that is, if we can assure that the method converges to a **stationary point**.
  - Introducing second order information, we can strengthen the result to include **convergence to a local minimum**.

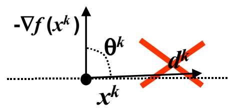
- Local convergence: how fast the sequence $\{x^k\}$ approaches to the optimal solution x^*.

Fundamentals:

Global convergence

- To ensure "global" convergence, several assumptions must be imposed to the objective function, the search direction and the steplength. Roughly speaking:
  - The objective f must be **bounded below** and **continuously differentiable**.
  - The gradient ∇f must be smooth (**Lipschitz continuous**).
  - The search direction d^k must be a **descent direction**.
  - The steplengths α^k must satisfy the **Wolfe conditions**.
  - The **angle** θ^k between the search directions d^k and the steepest descent direction $-\nabla f(x^k)$ must be **bounded away from 90°**

$$\cos\theta^k = \frac{-\nabla f(x^k) d^k}{\left\|\nabla f(x^k)\right\| \left\|d^k\right\|}$$



Fundamentals:

Conditions for "global" convergence

- **Zoutendijk's theorem:**

  *Consider any iteration of the form $x^{k+1} := x^k + \alpha^k d^k$ where d^k **is a descent direction** and α^k **satisfies the Wolfe conditions**. Suppose that f **is bounded below** in $\Re^n$ and that f **is continuously differentiable** in an open set N containing the level set*

$$L = \left\{ x : f(x) \le f(x^0) \right\}$$

  *where x^0 is the starting point of the iteration. Assume also that the **gradient is Lipschitz continuous** in N, that is, there exists a constant $L > 0$ such that:*

$$\left\| \nabla f(x) - \nabla f(\tilde{x}) \right\| \le L \left\| x - \tilde{x} \right\|, \quad \text{for all } x, \tilde{x} \in N$$

  Then

$$\sum_{k\ge 0} \cos^2\theta^k \left\| \nabla f(x^k) \right\|^2 < \infty \quad (\textit{Zoutendijk condition})$$

Fundamentals:

Interpretation of the Zoutendijk condition

- The Zoutendijk condition implies:

$$\cos^2\theta^k \left\|\nabla f(x^k)\right\|^2 \to 0 \qquad (1)$$

- If the method for choosing the search direction d^k ensures that the angle θ^k is bounded away from 90°, then there is a positive constant δ such that:

$$\cos\theta^k \geq \delta > 0 \quad \forall k$$

then, it follows from (1) that:

$$\lim_{k\to\infty}\left\|\nabla f(x^k)\right\| = 0$$

Fundamentals:

Linear and superlinear order of convergence

- **Linear convergence**:

*let $\{x^k\}$ be a sequence in $\Re^n$ that converges to x^*. We say that the convergence is **Q-linear** (or simply linear) if there is a constant $r\in(0,1)$ (ratio of convergence) such that*

$$\frac{\left\|x^{k+1}-x^*\right\|}{\left\|x^k-x^*\right\|} \leq r \quad \text{, for all } k \text{ sufficiently large}$$

- *The convergence is said to be **Q-superlinear** if*

$$\lim_{k\to\infty}\frac{\left\|x^{k+1}-x^*\right\|}{\left\|x^k-x^*\right\|} = 0$$

Fundamentals:

Quadratic order of convergence

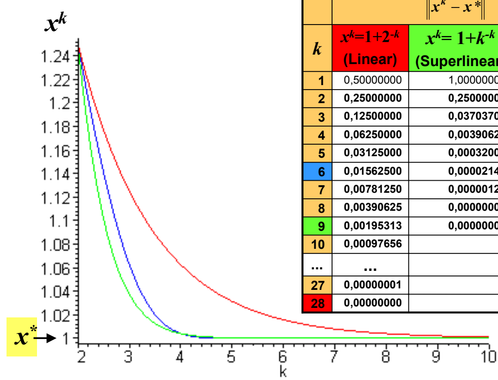
- **Quadratic convergence**:

*let $\{x^k\}$ be a sequence in $\Re^n$ that converges to x^*. We say that the convergence is **Q-quadratic** (or simply quadratic) if there is a constant $M>0$ such that :*

$$\frac{\left\|x^{k+1}-x^*\right\|}{\left\|x^k-x^*\right\|^2} \leq M \quad \text{, for all } k \text{ sufficiently large}$$

Fundamentals:

Order of convergence: example



k	$\left\|x^k - x^*\right\|$ $x^k=1+2^{-k}$ (Linear)	$x^k=1+k^{-k}$ (Superlinear)	$x^k=1+2^{-2^{k-1}}$ (Quadratic)
1	0,50000000	1,00000000	0,50000000
2	0,25000000	0,25000000	0,25000000
3	0,12500000	0,03703704	0,06250000
4	0,06250000	0,00390625	0,00390625
5	0,03125000	0,00032000	0,00001526
6	0,01562500	0,00002143	0,00000000
7	0,00781250	0,00000121	
8	0,00390625	0,00000006	
9	0,00195313	0,00000000	
10	0,00097656		
...	...		
27	0,00000001		
28	0,00000000		

Fundamentals
Order of convergence of the UNOP alg.

Algorithm	Order of convergence	
	f quadratic	f general
Steepest descent	Linear (r depends on $\nabla^2 f(x^*)$)	
Quasi-Newton	Superlinear	
Conjugate Gradients	$\leq n$ iterations	Quadratic (sub-sequence $\{x^{k+n}\}$)
Newton	1 iteration	Quadratic

Methods that use first derivatives
The Steepest Descent method (SD)

- **Search direction**: $d_{SD}^k = -\nabla f(x^k)'$
- **Global convergence:**
  - **Descent direction**: $\nabla f(x^k)\, d^k = -\|\nabla f(x^k)\| < 0$
  - **Zoutendijk condition**: angle $\theta^k = 0°$, $\cos(\theta^k) = 1\ \forall k$
- **Local convergence:**
  - Linear convergence.
  - The rate of convergence r depends on the properties of $f(x)$
- **Computational requirements:**
  - **Low memory requirements** : only needs to store several vectors of dimension n
  - Very easy to implement.

Methods that use first derivatives
Rate of convergence of the SD

- **Upper bound to the rate of convergence**

"Suppose that $f : \Re^n \to \Re$ is twice continuously differentiable, and that the iterates generated by the steepest descent method with exact line search converges to a point x^* where the Hessian matrix $\nabla^2 f(x^*)$ is positive definite. Then:

$$f(x^{k+1}) - f(x^*) \leq \beta\left[f(x^k) - f(x^*)\right] \ ; \ \beta = \left(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\right)^2$$

where $\lambda_1 \leq \ldots \leq \lambda_n$ are the eigenvalues of $\nabla^2 f(x^*)$ "

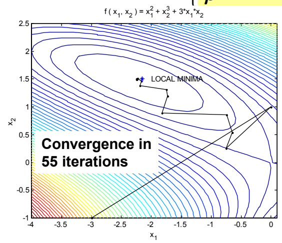
Methods that use first derivatives
Rate of convergence of the SD: example

- ***f(x)* with "slow" rate of conv.**

$$f(x_1, x_2) = x_1^2 + x_2^3 + 3x_1x_2$$

$$x^0 = [-3 \quad -1]' \quad x^* = [-2.25 \quad 1.5]'$$

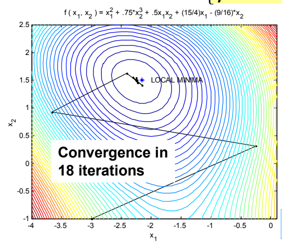
$$\nabla^2 f(x^*) = \begin{bmatrix} 2 & 3 \\ 3 & 9 \end{bmatrix} \ ; \ \begin{cases} \lambda_1 = 0.8902 \\ \lambda_2 = 10.1098 \\ \beta = 0.7025 \end{cases}$$



- ***f(x)* with "fast" rate of conv.**

$$f(x_1, x_2) = x_1^2 + \tfrac{3}{4}x_2^3 + \tfrac{1}{2}x_1x_2 + + \tfrac{15}{4}x_1 - \tfrac{9}{16}x_2$$

$$\nabla^2 f(x^*) = \begin{bmatrix} 2 & .5 \\ .5 & 2.25 \end{bmatrix} \ ; \ \begin{cases} \lambda_1 = 1.6096 \\ \lambda_2 = 2.6404 \\ \beta = 0.0588 \end{cases}$$



Methods that use first derivatives

The Conjugate Gradient method (CG)

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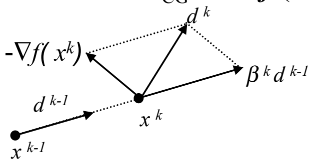
- **Search direction:** $d_{\mathrm{CG}}^{k} = -\nabla f(x^{k})' + \beta^{k} d^{k-1}$



- **Choices of β^k:**

Fletcher-Reeves : $\beta_{\mathrm{FR}}^{k} = \dfrac{\nabla f(x^{k})\nabla f(x^{k})'}{\left\|\nabla f(x^{k-1})\right\|^{2}}$

(best theoretical prop.)

Polak-Ribière : $\beta_{\mathrm{PR}}^{k} = \dfrac{\nabla f(x^{k})\left(\nabla f(x^{k}) - \nabla f(x^{k-1})\right)'}{\left\|\nabla f(x^{k-1})\right\|^{2}}$

(best practical behaviour)

Unconstrained Nonlinear Optimization

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Methods that use first derivatives

Properties of the CG method (I)

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- **Global convergence** :
  - **Descent direction**: d^k_{GC} is a descent direction if the steplength α^k satisfies the *strong Wolfe conditions* :

$$f(x^k + \alpha d^k) \le f(x^k) + [c_1 \nabla f(x^k) d^k]\alpha \quad \text{(SW1)}$$
$$\left|\nabla f(x^k + \alpha d^k) d^k\right| \le c_2 \left|\nabla f(x^k) d^k\right| \quad \text{(SW2)}$$
$$0 < c_1 < c_2 < \tfrac{1}{2}$$

  - **Zoutendijk condition** : can be proved if the method is periodically restarted setting:

$$d_{\mathrm{CG}}^{l} = -\nabla f(x^{l})' = d_{\mathrm{SD}}^{l} \;,\; l = n, 2n, 3n, \ldots$$

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Methods that use first derivatives

Properties of the CG method (II)

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- **Local convergence** :
  - The CG method with restart has ***n*-step quadratically** convergence, that is:

$$\left\|x^{k+n} - x^*\right\| = O\left(\left\|x^{k} - x^*\right\|^{2}\right)$$

- **Computational requirements** :
  - **Low memory consumption**: only needs to store several vectors of dim n.
  - Almost as simple to implement as SD (the only difficulty is the computation of constant β^k).

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Methods that use first derivatives

Example of the CG method

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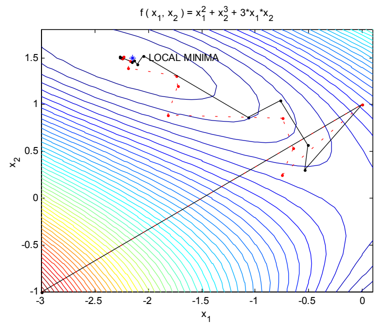
- **Exemple** : $f(x_1, x_2) = x_1^{\,2} + x_2^{\,3} + 3x_1x_2$

$x^0 = [-3 \;\; -1]' \qquad x^* = [-2.25 \;\; 1.5]'$



CG method (38 iterations)

SD method (55 iterations)

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Methods that use first derivatives

Quasi-Newton methods (QN)

- **Rationale of the Newton method**:
  To find the next iterate x^{k+1} as the minimizer of the quadratic model $m^k(p)$ of $f(x)$ around the current iterate x^k:

$$f(x^k+p) \approx f(x^k) + \nabla f(x^k)p + \frac{1}{2}p'\nabla^2 f(x^k)p \equiv m^k(p)$$

$$p^k \leftarrow \operatorname{argmin}\{m^k(p)\}$$

$$\nabla m^k(p^k) = \nabla^2 f(x^k)p^k + \nabla f(x^k)' = 0 \rightarrow p^k = -\nabla^2 f(x^k)^{-1}\nabla f(x^k)$$

$$x^{k+1} = x^k + p^k$$

- **Quasi-Newton method**:
  Applies a Newton strategy *avoiding the need of second derivatives* by substituiting the Hessian matrix $\nabla^2 f(x^k)$ by an approximation B^k

Methods that use first derivatives

Quasi-Newton methods (QN)

- **Quasi-Newton direction:** $d^k_{\text{QN}} = -\left[B^k\right]^{-1}\nabla f(x^k)'$
- **Choices of B^k**: given a symmetric pos. def. matrix B^0 , and: $s^k = x^{k+1} - x^k$; $y^k = \nabla f(x^{k+1})' - \nabla f(x^k)'$

Broyden-Fletcher-Goldfarb-Shanno (BFGS) :

$$B^{k+1}_{\text{BFGS}} = B^k_{\text{BFGS}} - \frac{B^k_{\text{BFGS}} s^k {s^k}^T B^k_{\text{BFGS}}}{{s^k}^T B^k_{\text{BFGS}} s^k} + \frac{y^k {y^k}^T}{{y^k}^T s^k}$$

Davidon-Fletcher-Powell (DFP) : $H^k = [B^k]^{-1}$

$$H^{k+1}_{\text{DFP}} = H^k_{\text{DFP}} - \frac{H^k_{\text{DFP}} y^k {y^k}^T H^k_{\text{DFP}}}{{y^k}^T H^k_{\text{DFP}} y^k} + \frac{s^k {s^k}^T}{{y^k}^T s^k}$$

Methods that use first derivatives

Quasi-Newton methods (QN)

- The BFGS formula is considered to be the most effective of all quasi-Newton updating formulae.
- **Properties of matrix B^{k+1}** : given B^k, $n\times n$ symetric, positive definite matrix, then the BFGS update provides B^{k+1} that :
  - Is symetric
  - Is positive definite if $s^{k\prime} y^k > 0$.
    (guaranteed if α^k satisfies the Wolfe conditions)
  - Satisfies the ***secant equation*** : $B^{k+1}s^k = y^k$
    (this is how we force $B^{k+1} \approx \nabla^2 f(x^{k+1})$.)

Methods that use first derivatives

Global convergence of the BFGS method

- **Global convergence** :
  - **Descent direction**: we check the descent condition:

$$\left.\begin{array}{l} \nabla f(x^k)d^k_{\text{BFGS}} = -\nabla f(x^k)\left[B^k_{\text{BFGS}}\right]^{-1}\nabla f(x^k)' \\ B^k_{\text{BFGS}} \text{ pos. def.} \Rightarrow \left[B^k_{\text{BFGS}}\right]^{-1} \text{ pos. def} \end{array}\right\} \nabla f(x^k)d^k_{\text{BFGS}} < 0$$

  - **Zoutendijk condition** : can be proved if the matrices B^k have an uniformly bounded condition number, that is, if there is a constant M such that:

$$\operatorname{cond}(B^k) = \left\|B^k\right\|\left\|{B^k}^{-1}\right\| \leq M, \quad \text{for all } k$$

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Methods that use first derivatives

Local convergence of the BFGS method

- **Local convergence** : under the following assumptions:
  - *The objective function f is twice continuously differentiable*
  - *The level set $\Omega=\{\, x\in\Re^n : f(x) \le f(x^0) \,\}$ is convex*
  - *The objective function f has a unique minimizer x^* in Ω*
  - *The Hessian matrix $\nabla^2 f(x^{k+1})$ is Lipschitz continuous at x^* and positive definite on Ω.*

  It can be shown that the iterates generated by the BFGS algorithm converges superlinearly to the minimizer x^*

Unconstrained Nonlinear Optimization

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Methods that use first derivatives

Local convergence of the BFGS method

- **Computational issues** :
  - The efficient implementation of the BFGS method does not store B^k explicitily, but the Cholesky factorization:
    $$B^k = L^k D^k L^{k'}$$
  - **Memory consumption**: $n(n+1)/2$ = O(n^2) elements of the Cholesky factors.
  - **Computational cost per iteration** : O(n^2) operations necessary to ...

    ... update the Cholesky factors .

    ... find the solution of the linear system $B^k d^k = -\nabla f(x^k)$.
  - The development of an efficient implementation of the BFGS method is quite difficult.

Unconstrained Nonlinear Optimization

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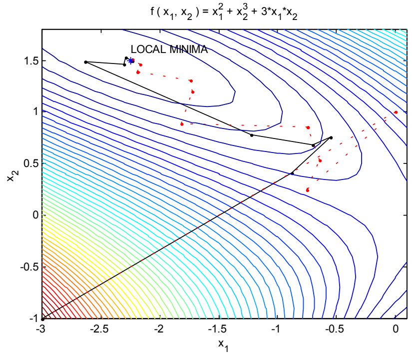
Methods that use first derivatives

Example of the BFGS method

- **Exemple** : $f(x_1,x_2)=x_1^{\,2}+x_2^{\,3}+3x_1x_2$

$x^0=[-3 \quad -1]'$

$x^*=[-2.25 \quad 1.5]'$



BFGS
(11 iterations)

SD method
(55 iterations)

Unconstrained Nonlinear Optimization

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Methods that use first and second derivatives

The Newton method (N)

- **Rationale of the Newton method:**

  To find the next iterate x^{k+1} as the minimizer of the quadratic model $m^k(p)$ of $f(x)$ around the current iterate x^k:

$$f(x^k+p) \approx f(x^k)+\nabla f(x^k)p+\frac{1}{2}p'\nabla^2 f(x^k)p \equiv m^k(p)$$

$$p^k \leftarrow \operatorname{argmin}\{m^k(p)\} = -\left[\nabla^2 f(x^k)\right]^{-1}\nabla f(x^k)$$

$$x^{k+1} = x^k + p^k$$

Unconstrained Nonlinear Optimization

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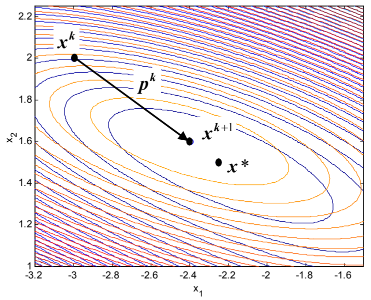
Methods that use first and second derivatives

The Newton method (N)

- **Exemple** : $f(x_1,x_2)=x_1^{\,2}+x_2^{\,3}+3x_1x_2$ $\quad x^k=[-3 \quad 2]'$

  $m^k(x_1,x_2)=x_1^{\,2}+6x_2^{\,2}+3x_1x_2-12x_2+21$



$$x^*=\begin{bmatrix}-2.25\\1.5\end{bmatrix}$$

(minimizer of f)

$$p^k=-\left[\nabla^2 f(x^k)\right]^{-1}\nabla f(x^k)=\begin{bmatrix}0.6\\-0.4\end{bmatrix}$$

$$x^{k+1}=x^k+p^k=\begin{bmatrix}-2.4\\1.6\end{bmatrix}$$

(minimizer of m^k)

Methods that use first and second derivatives

The Newton method (N)

- **Search direction:** $d_N^k=-\nabla^2 f(x^k)^{-1}\nabla f(x^k)^T$
- **Global convergence** :
  - **Descent direction**: the descent nature of d^k_N ***can only be guaranteed if*** the Hessian matrix $\nabla^2 f(x^k)$ is ***positive definite***:

    $$\text{If } \nabla^2 f(x^k) \text{ pos. def. then}$$
    $$\nabla f(x^k)d_N^k=-\nabla f(x^k)\nabla^2 f(x^k)^{-1}\nabla f(x^k)^T<0$$

    otherwise, ***the global convergence of the Newton method cannot be guaranteed***.

Methods that use first and second derivatives

Losing of the global convergence

- **Example** : $f(x_1,x_2)=x_1^{\,2}+x_2^{\,3}+3x_1x_2$

  Over x^0 = [-3 -1]', the Hessian matrix is:

  $$\nabla^2 f(x^0)=\begin{bmatrix}2 & 3\\3 & -6\end{bmatrix}$$

  which is indefinite (λ_1=3, λ_2=-7). Therefore, the descent property of the Newton direction cannot be guaranteed.In fact, after 1 iteration, the method finds an ascent direction:

k	$\nabla^2 f(x^k)$	$\nabla f(x^k)\ d_N^k$	
0	Indefinite	$-35.1428 < 0$	Descent direction
1	Indefinite	$0.37699 > 0$	ASCENT direction

Methods that use first and second derivatives

Local convergence of the Newton method

- **Local convergence** :

  "Suppose that
  - *The solution x^* satisfies the sufficient optimality condition .*
  - *The function f is twice differentiable.*
  - *The Hessian $\nabla^2 f(x)$ is Lipschitz continuous in a neighbourhood of a solution x^**

  Consider the Newton iteration $x^{k+1}=x^k+d_N^k$. Then:
  - *if the starting point x^0 is sufficiently close to x^*, the sequence of iterates converges to x^*;*
  - *the order of convergence of $\{x^k\}$ is quadratic; and*
  - *the sequence of gradient norms $\{\|\nabla f(x^k)\|\}$ converges quadratically to zero."*

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Methods that use first and second derivatives

Quadratic order of convergence

- **Example :** $f(x_1, x_2) = x_1^2 + x_2^3 + 3x_1x_2$

  The newton method converges from x^0 = [-3 2]' to x^*=[-2.25 1.5]^T in 4 iterations, **reducing the error $\|x^k - x^*\|$ quadratically** at each step :

k	$\|x^k-x^*\|$	$\le$	$\|x^{k-1}-x^*\|^2$	$\|\nabla f(x^k)\|$
0	9.013×10^{-1}			3.0
1	1.803×10^{-1}	$\le$	8.125×10^{-1}	4.8×10^{-1}
2	1.060×10^{-2}	$\le$	3.250×10^{-2}	2.657×10^{-2}
3	4.126×10^{-5}	$\le$	1.124×10^{-4}	1.029×10^{-4}
4	6.296×10^{-10}	$\le$	1.702×10^{-9}	1.571×10^{-9}

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Methods that use first and second derivatives

Modified Newton methods (MN)

- **Search direction:**

$$d^k_{\mathrm{MN}} = -{B^k_{\mathrm{MN}}}^{-1} \nabla f(x^k)^T$$

where $B^k_{\mathrm{MN}} = \nabla^2 f(x^k) + E^k$, with

  - $E^k = 0$ if $\nabla^2 f(x^k)$ is sufficiently positive definite;
  - otherwise E^k is chosen to ensure that B^k_{MN} is sufficiently positive definite.

- **Methods to compute B^k_{MN}** : based on the modification of
  - The *spectral decomposition* of $\nabla^2 f(x^k) = Q\Lambda Q^T$.
  - The *Cholesky factorization* of $\nabla^2 f(x^k) = LDL^T$.

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Methods that use first and second derivatives

Global convergence of the MN method

- **Global convergence** :
  - **Descent direction**: as B^k_{MN} is always positive definite,therefore, d^k_{MN} is a descent search direction.
  - **Zoutendijk condition** : can be proved if the matrices B^k_{MN} have an uniformly bounded condition number, that is, if there is a constant M such that :

$$\mathrm{cond}(B^k_{\mathrm{MN}}) = \left\| B^k_{\mathrm{MN}} \right\| \left\| {B^k_{\mathrm{MN}}}^{-1} \right\| \le M, \quad \text{for all } k$$

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Methods that use first and second derivatives

Local convergence of the MN method

- **Local convergence** :
  - If the sequence of iterates $\{x^k\}$ converges to a point x^* where $\nabla^2 f(x^*)$ is sufficiently positive definite (i.e. $E^k = 0$ for k large enough), then the MN method reduces to the Newton methods, and the convergence is quadratic.
  - If $\nabla^2 f(x^*)$ is close to singular (that is, there is not guarantee that E^k=0) the convergence rate may only be linear.

Unconstrained Nonlinear Optimization

Methods that use first and second derivatives

Other aspects of the MN methods

- **Computational issues** :
  - The efficient implementation of the MN methods computes and store the modified Cholesky factorization of B^k_{MN}.
  - **Memory consumption**: $n(n+1)/2$ = O(n^2) elements of the Cholesky factors.
  - **Computational cost per iteration** : O(n^3) operations necessary to ...

    ... compute the modified Cholesky factors of $\nabla^2 f(x^*)$.

    ... find the solution of the linear system $B^k_{MN}\, d^k_{MN} = -\nabla f(x^k)$

    plus the effort of computing the second derivatives
  - The efficient implementation of the MN method is quite difficult.

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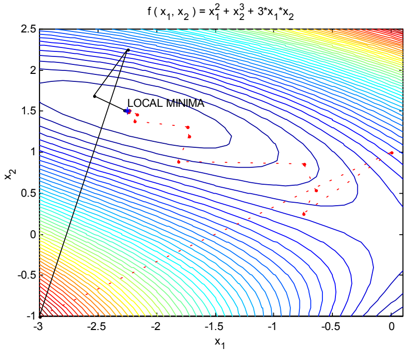
Methods that use first and second derivatives

Example of MN method (modified Chol. fac.)

- **Example** : $f(x_1,x_2)=x_1^{\,2}+x_2^{\,3}+3x_1x_2$ $\quad x^0=[-3\quad -1]'$ $\quad x^*=[-2.25\quad 1.5]'$



MN method (4 iterations)

SD method (55 iterations)

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Unconstrained Nonlinear Optimization

Nonderivative methods

Motivation and classification

- **Motivation:** in many problems, either the derivatives are not available in explicit form or they are given by very complicated expressions, prone to produce coding errors.
- **Example:** a Log-Likelihood function like

$$
\begin{aligned}
l(\breve{u},\alpha,\beta,\sigma)=\sum_{i=1}^{n}\Bigg[&\varepsilon_i\xi_{1i}\ln\left(\sum_{j=1}^{m}\frac{\gamma_{ij}}{\sigma}\exp\left[\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}-e^{\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}}\right]\omega_j\right)\\
&+\varepsilon_i\xi_{2i}\ln\left(\sum_{j=1}^{m}\gamma_{ij}\exp\left[-e^{\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}}\right]\omega_j\right)\\
&+\varepsilon_i(1-\xi_{1i})(1-\xi_{2i})\ln\left(\sum_{j=1}^{m}\gamma_{ij}\left(1-\exp\left[-e^{\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}}\right]\right)\omega_j\right)+(1-\varepsilon_i)\ln\left(\sum_{j=1}^{m}\gamma_{ij}\omega_j\right)\Bigg]
\end{aligned}
$$

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Nonderivative methods

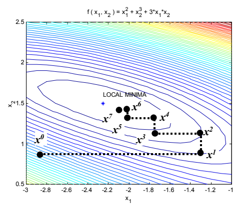
Classification

- **Finite differences** : to use a first derivative method (SD,CG,QN), computing the gradient as:

$$\frac{\partial f(x^k)}{\partial x_i}\approx\frac{1}{\varepsilon}\left(f(x^k+\varepsilon e_i)-f(x^k)\right)$$

  with ε a small positive scalar and e_i the unit vector

- **Coordinate descent:** the obj. function is minimized along one coordinate direction at each iteration.

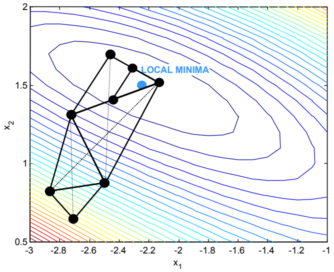


Nonderivative methods

Classification

– **Nelder & Mead simplex method** :

– Not to be confused with the simplex method for linear programming.

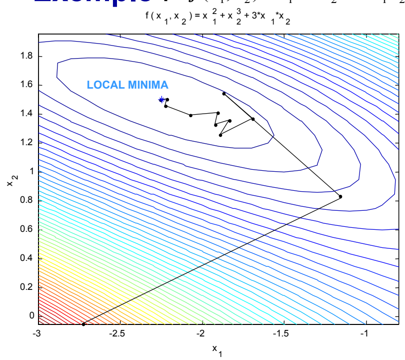


- Start with an initial **simplex** (convex hull of $n+1$ points).
- Select a new point that improves the worst point of the current simplex.
- Update de current simplex.

Nonderivative methods

Nelder & Mead method

- **Exemple** : $f(x_1,x_2)=x_1^2+x_2^3+3x_1x_2$ $\quad x^*=[-2.25 \quad 1.5]^t$



NM method (11 iterations)

Methods for Unconstrained Nonlinear Optimization

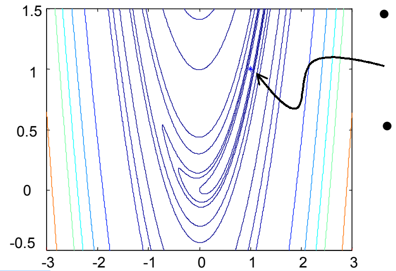
Computational comparison

Rosenbrock function (n=4)	Iter.	Execution time (seconds)	$f(x^*)$	$\|\| \nabla f(x^*) \|\|$
Steepest Descent	4760	120.34	1.038×10^{-11}	9.222×10^{-6}
Nelder & Mead	222	3.84	4.586×10^{-12}	8.828×10^{-5}
Conjugate Gradient	42	1.43	7.513×10^{-13}	7.820×10^{-7}
Quasi-Newton	27	0.33	4.980×10^{-17}	2.793×10^{-7}
Modified Newton	14	0.22	3.344×10^{-26}	2.506×10^{-12}
Newton	14	0.16	3.344×10^{-26}	2.506×10^{-12}

The extended Rosenbrock function

$$f(x)=\sum_{i=1}^{n/2}\left[10\left(x_{2i}-x_{2i-1}^2\right)^2+\left(1-x_{2i-1}\right)^2\right]$$

The contours lines for $n=2$:



- Unique global minimizer at $x^*=[\ 1\ \ 1\ ]^T$
- It is considered a difficult function to minimize.

Nonlinear Least-Squares Problems

- We will study now the solution for the Nonlinear Least-Squares Problem

$$\text{(NLSP)} \quad \min_{x \in \Re^n} f(x) = \frac{1}{2} \sum_{j=1}^{m} r_j^2(x) = \frac{1}{2} \| r(x) \|_2^2$$

where $r_j(x)$ represents the residuals of the model to be adjusted, and the decision variables x are the coefficients of the model.

Nonlinear Least-Squares Problems

- For instance, in the SIDS model:

$$\min_{\substack{a_i, b_i, c_i \\ i=1,2,\ldots,5}} \frac{1}{2} \sum_{i=1}^{5} \sum_{k=1}^{365} \left[t_{ik}(a_i, b_i, c_i) - t_{ik} \right]^2$$

we have:

- Decision variables: $x = [a_i \quad b_i \quad c_i]_{i=1,2,\ldots,5} \in \Re^{15}$
- Residuals: $r_j(x) = t_{ik}(a_i, b_i, c_i) - t_{ik}$
- Objective function:

$$f(x) = \frac{1}{2} \sum_{i=1}^{5} \sum_{k=1}^{365} \left[t_{ik}(a_i, b_i, c_i) - t_{ik} \right]^2$$

NLSP through the Newton method

- Remember that the **Newton search direction** was defined as :

$$d_N^k = -\nabla^2 f(x^k)^{-1} \nabla f(x^k)^T$$

therefore, in order to solve the NLSP with the Newton method, we need the **first and second derivatives of the objective function**

$$f(x) = \frac{1}{2} \sum_{j=1}^{m} r_j^2(x)$$

NLSP through the Newton method

- The derivatives of $f(x)$ can be expressed in terms of the **Jacobian of the residuals r**:

$$J(x) = \left[\frac{\partial r_j}{\partial x_i} \right]_{\substack{j=1,2,\ldots,m \\ i=1,2,\ldots,n}}$$

The gradient is: $\nabla f(x) = \sum_{j=1}^{m} r_j(x) \nabla r_j(x) = J(x)^T r(x)$

and the Hessian :

$$\nabla^2 f(x) = \sum_{j=1}^{m} \nabla r_j(x) \nabla r_j(x)^T + \sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x) =$$

$$= J(x)^T J(x) + \sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x)$$

The Gauss-Newton (G-N) method (I)

- The **Gauss-Newton** method applies a **Newton** method to the NLSP, **substituting the true Hessian**

A

$$\nabla^2 f(x) = J(x)^T J(x) + \sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x)$$

by the approximation that neglects the term **A** : $\nabla^2 f(x) \approx J(x)^T J(x)$

,that is the **Gauss-Newton search direction** is :

$$d^K_{\text{G-N}} = -\left[J(x^k)^T J(x^k)\right]^{-1} J(x^k)^T r(x^k)$$

The G-N method (II)

- **Considerations**: the approximation $\nabla^2 f(x) \approx J(x)^T J(x)$ is appropiate when the term $J(x)^T J(x)$ dominates over $\sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x)$ in the expression of the Hessian. This happends:
  - when the residuals r_j are small.
  - when each r_j is nearly a linear function, so that $\|\nabla^2 r_j(x)\|$ is small.

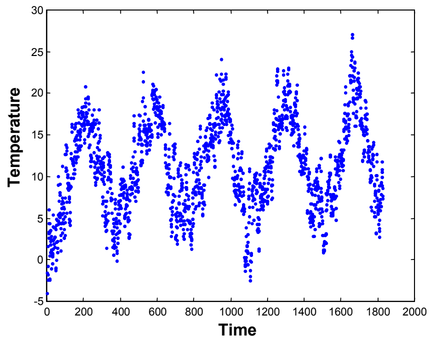
The G-N method (III)

- **Advantages**:
  - There is **no need to compute** the second derivatives $\nabla^2 r_j(x)$.
  - The G-N method can be shown to be **globally convergent** under certain conditions over the rank of $J(x^k)$.
  - The speed of convergence depends on how much the leading term $J(x)^T J(x)$ dominates.

  When $\sum_{j=1}^{m} r_j(x^*) \nabla^2 r_j(x^*) = 0$ the convergence is quadratic.

Example: the SIDS problem

- Real data (high dispersion):



Nonlinear Least-squares problems

Example: the SIDS problem, large residuals

- The residuals at the optimal solution are large:

  $\| r(x^*) \|_2 = 117.105, \quad \| r(x^*) \|_\infty = 8.280$

  nevertheless, the approximation $\nabla^2 f(x^k) \approx J(x^k)^T J(x^k)$ is very good near the solution:

  $\| \nabla^2 f(x^0) - J(x^0)^T J(x^0) \|_F = 1665.46$

  $\| \nabla^2 f(x^*) - J(x^*)^T J(x^*) \|_F = 4.129\times10^{-5}$

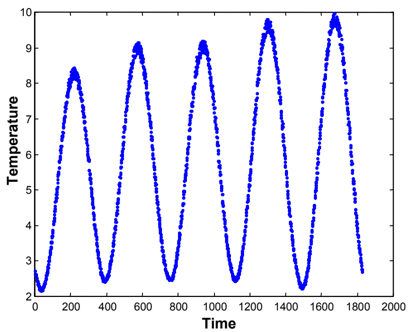
SIDS, large residuals	Exec. time (seconds)	$f(x^*)$	$\|\nabla f(x^*)\|$
Steep. Descent	42.90	6856.886	2.899×10^{-3}
Quasi-Newton	20.15	6856.886	1.192×10^{-4}
Gauss-Newton	16.63	6856.886	2.564×10^{-5}
Modified Newton	3.07	6856.886	9.524×10^{-5}

Graph

Nonlinear Least-squares problems

Example: the SIDS problem, small residuals

- Simulated data with low dispersion:



Nonlinear Least-squares problems

Example: the SIDS problem, small residuals

- The residuals are small:

  $\| r(x^*) \|_2 = 3.108, \ \| r(x^*) \|_\infty = 0.190$

- The approximation $\nabla^2 f(x^k) \approx J(x^k)^T J(x^k)$ is very good near the solution:

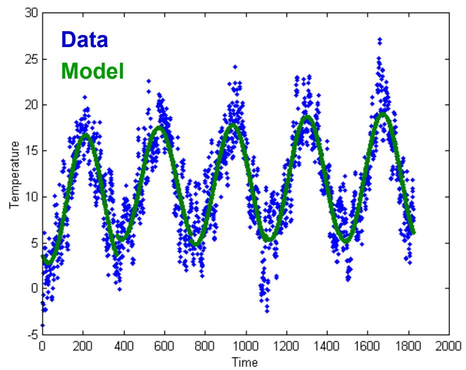
  $\| \nabla^2 f(x^0) - J(x^0)^T J(x^0) \|_F = 849.169$

  $\| \nabla^2 f(x^*) - J(x^*)^T J(x^*) \|_F = 5.813\times10^{-7}$

SIDS, small residuals	Exec. time (seconds)	$f(x^*)$	$\|\nabla f(x^*)\|$
Steep. Descent	18.34	4.832	3.209×10^{-6}
Quasi-Newton	15.49	4.832	7.137×10^{-7}
Gauss-Newton	16.81	4.832	4.912×10^{-7}
Modified Newton	3.25	4.832	5.689×10^{-9}

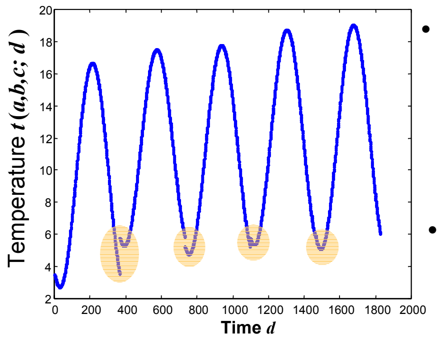
Nonlinear Least-squares problems

Solution for the SIDS problem



Nonlinear Least-squares problems

Adjusted model for temperature



- The adjusted model for the temperature presents discontinuities in the connecting points between different years.
- This problem can be avoided by **introducing constraints on the SIDS problem**

Algorithms for Constrained Nonlinear Optimization

Constrained Nonlinear Optimization

Fundamentals:

Formulation of the NOP

- The general (standard) form of the NOP is :

$$(\text{NOP})\begin{cases}\min\limits_{x\in\Re^n} & f(x) & \textbf{Objective function}\\ \text{subject to:} & h(x)=0 & \textbf{Equality constraints}\\ & g(x)\le 0 & \textbf{Inequality constraints}\end{cases}$$

where x are the **decision variables**, or simply, **variables**, and

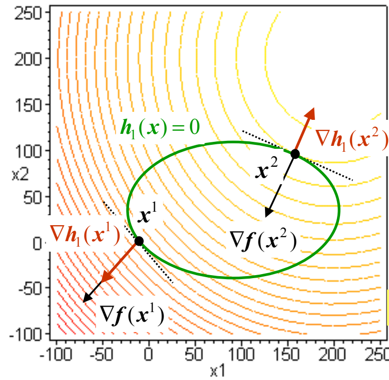
$$f:\Re^n\to\Re \qquad h:\Re^n\to\Re^m \qquad g:\Re^n\to\Re^l$$

- (NOP) will also be expressed as:

$$(\text{NOP})\ \min_x\{f(x)\mid x\in X\}\ ;\ \ X=\{x\in\Re^n\mid h(x)=0,\ g(x)\le 0\}$$

Fundamentals:

Geometry of the optimality conditions (I)

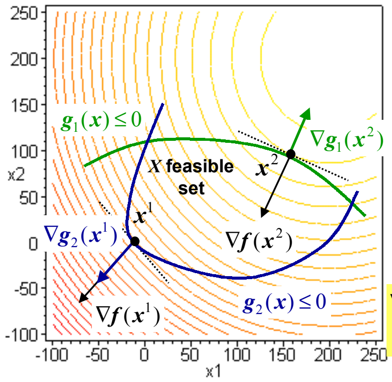


- One equality constraint
- Two stationary points x^1 and x^2 (x^2 minimum if f convex.)
- Relation between $\nabla f(x^k)$ and $\nabla h_1(x^k)$ at x^k, stationary point:

$$\nabla f(x^k)+\lambda_1\nabla h_1(x^k)=0$$

Fundamentals:

Geometry of the optimality conditions (II)



- Two inequality constraints defining X
- One stationary point, x^2 (x^1 is no longer stationary)
- Relation between $\nabla f(x^k)$ and $\nabla g_j(x^k)$ at x^k, stationary point:

$$\nabla f(x^k) + \mu_j \nabla g_j(x^k) = 0$$
$$\boxed{\mu_j \ge 0}$$

for all g_j active at x^k

Fundamentals:

Optimality conditions : the KKT conditions

Usual stopping criterium

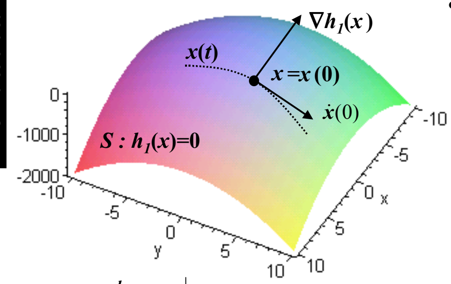
- **First-Order Necessary Conditions**
  "*Suppose that x^* is a local minimizer of NOP and that x^* is* regular, *then there are Lagrange multipliers vectors $\lambda \in \Re^m$ and $\mu \in \Re^l$ such that :*

$$i) \quad \nabla f(x^*) + \lambda^{*T} \nabla h(x^*) + \mu^{*T} \nabla g(x^*) = 0$$
$$ii) \quad \mu^{*T} g(x^*) = 0$$
$$iii) \quad \mu^* \ge 0$$

- This are the famous **Karush-Kuhn-Tucker conditions** (**KKT** for short).

Fundamentals:

Another interpretation of the KKT conditions



- Consider one equality constraint and a feasible point x
- Let $x(t)$ be *differentiable curve* over the feasible surface S at x.
- The derivative of $x(t)$ at t=0 is:

$$\dot{x}(0) = \frac{d}{dt} x(t)\Big|_{t=0}$$

- Then : $\frac{d}{dt} f(x(t))\Big|_{t=0} = \nabla f(x)\dot{x}(0)$. The **KKT** conditions impose that, **if x is a minimizer, this derivative must be nonnegative for all possible diff. curves $x(t)$.**

Fundamentals:

Optimality conditions

- **Regularity condition:**
  any feasible point $x \in X$ is said to be regular if the gradient vectors:

$$\nabla h_i(x) \quad , \quad i = 1,2,\ldots,m$$
$$\nabla g_j(x) \quad , \quad j \in J = \{ j \mid g_j(x) = 0 \}$$

Active constraints

are linearly independent.

Motivation

- Remember the likelihood maximization problem introduced previously:

$$\text{(LCNOP)}\quad \begin{cases} \max\limits_{\substack{\grave{u}\in\Re^m\\ \alpha,\beta,\sigma}} & L_n(\grave{u},\alpha,\beta,\sigma)=\prod\limits_{i=1}^{n}\sum\limits_{j=1}^{m}\gamma_{ij}\dfrac{1}{\sigma\sqrt{2\pi}}\left(e^{-\frac{1}{2}\frac{(y_i-\alpha-\beta s_j)^2}{\sigma^2}}\right)\omega_j \\ \text{subject to:} & \sum\limits_{j=1}^{m}\omega_j=1 \\ & \omega_j\ge 0,\ j=1,\dots,m \\ & \sigma\ge 0 \end{cases}$$

This is an exemple of *Linearly Constrained NOP Problem (LCNOP).*

- We will use the Reduced Gradient method to illustrate the rationale of the algorithms for (LCNOP).

The Reduced Gradient (RG) method

- The Reduced Gradient method solves the (LCNOP) problem:

$$\text{(LCNOP)}\ \min_x\{f(x)|x\in X\}\ ;\ X=\{x\in\Re^n|Ax=b, l\le x\le u\}$$

using the following strategy:

1. Find a first feasible solution $x^k\in X$ (current solution).

2. If the current solution satisfies the KKT conditions, x^k, STOP

3. Otherwise, find a new feasible solution that improves the current objective function value, and take this new point as the current solution:

- **3.1.** Find a **feasible descent** search direction d^k
- **3.2.** Perform a linesearch from x^k along d^k : α^k
- **3.3.** Update the current solution: $x^{k+1} := x^k + \alpha^k d^k$. Goto 2

Feasible direction

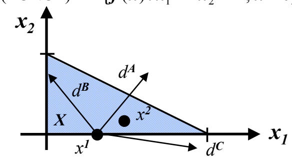
- **Feasible direction :** $d^k\in\Re^n$ is a feasible direction at x^k for the problem

$$\text{(LCNOP)}\ \min_x\{f(x)|x\in X\}\ ;\ X=\{x\in\Re^n|Ax=b, l\le x\le u\}$$

If :

$$\exists\bar{\alpha}\in\Re^+\,|\,\forall\alpha\in[0,\bar{\alpha}]: x^k+\alpha d^k\in X$$

$$\text{(LCNOP)}\min\{f(x): x_1+2x_2\le 2,\ x\ge 0\}$$



Over x^1 :	Over x^2 :
d^A: FEASIBLE d^B: FEASIBLE	$\forall d\in\Re^n$ FEASIBLE
d^C: INFEASIBLE	

Feasible descent direction of the RG

- **Nondegeneracy assumption:** at each iterate x^k, the RG method assumes that there exists a partition of the variables and columns of the coefficient matrix A:

$$x^k=\left[\frac{y}{z}\right]\quad \begin{array}{ll} y\in\Re^m & \text{(dependent variables)}\\ z\in\Re^{n-m} & \text{(independent variables)}\end{array}$$

$$Ax=[A_y\ |\ A_z]\left[\frac{y}{z}\right]=A_y y+A_z z=b$$

such that:

$$\begin{array}{ll} i. & A_y\in\Re^{m\times m}\ \text{is non-singular}\\ ii. & l_y<y<u_y\end{array}$$

Linearly constrained NOP

Feasible descent direction of the RG

- **Reduced gradient**: given the partition $x^k=[y\ z]^T$, the reduced gradient is the vector $r\in\Re^{n-m}$ defined as:

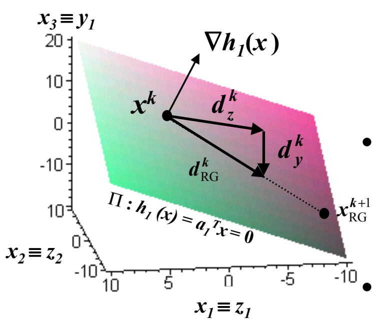
$$r^T = \nabla_z f(y,z) - \nabla_y f(y,z) A_y^{-1} A_z$$

- **Search direction**: it is obtained after the reduced gradient as:

$$d_{\mathrm{RG}}^k = \begin{bmatrix} d_y^k \\ d_z^k \end{bmatrix} = \begin{bmatrix} -A_y^{-1}A_z(-r) \\ \hline -r \end{bmatrix}$$

Linearly constrained NOP

Geometrical interpretation of d^k_{RG}



- Consider one linear constraint $a_1^T x = 0$ defining the feasible plane Π, and the feasible point x^k, where $z=[x_1\ x_2]^T$ and $y=x_3$
- The step d_z^k moves away from Π...

  ... and the step d_y^k corrects the step so that d^k_{RG} lies in Π
- And finally, a linesearch is performed to find x^{k+1}

Linearly constrained NOP

Feasible descent direction of the RG

- **Properties of d^k_{RG}:**
  - **d^k_{RG} is a descent direction**:

$$\nabla f(x^k) d_{RG}^k = [\nabla_y f(y,z) \mid \nabla_z f(y,z)] \begin{bmatrix} -A_y^{-1}A_z(-r) \\ \hline -r \end{bmatrix} =$$
$$= -\nabla_y f(y,z) A_y^{-1} A_z (-r) + \nabla_z f(y,z)(-r) =$$
$$= \underbrace{[\nabla_z f(y,z) - \nabla_y f(y,z) A_y^{-1} A_z]}_{r}(-r) = -r^T r =$$
$$= -\|r\| < 0 \quad \text{if} \quad r \neq 0$$

  - **d^k_{RG} is feasible for $Ax=b$:**

$$A(x^k + \alpha d_{RG}^k) = b + \alpha [A_y \mid A_z] \begin{bmatrix} -A_y^{-1}A_z(-r) \\ \hline -r \end{bmatrix} = b + \alpha \overbrace{\begin{bmatrix} -\overbrace{A_y A_y^{-1}}^{I} A_z + A_z \end{bmatrix}}^{0}(-r) = b$$

Linearly Constrained NOP

Feasible descent direction of the RG

- **Properties of d^k_{RG} (cont.):**
  - **d^k_{RG} may be infeasible for some bound**:

    this problem can be avoided by a slightly modification in the definition of the search direction.

Motivation : nonlinear regression with constraints

- Remember the SIDS problem

$$\min_{\substack{a_i, b_i, c_i \\ i=1,2,\ldots,5}} \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{365} \left[t_{ij}(a_i, b_i, c_i) - t_{ij} \right]^2$$

where the model to be adjusted was:

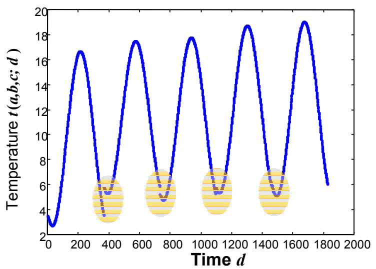
$$t_{ij}(a_i, b_i, c_i) = a_i \cos\left(\frac{2\pi}{365} j - b_i \right) + c_i$$

$$i = 1,2,3,4,5$$

$$j = 1,2,\ldots,365$$

Motivation : nonlinear regression with constraints

- The solution of this problem through unconstrained nonlinear optimization techniques presented discontinuities between the harmonic models for each year:



Motivation : nonlinear regression with constraints

- This problem can be overcame by introducing a set of **nonlinear constraints** that forces the continuity of the adjusted models:

$$h_i(x) = t_{i365}(a_i, b_i, c_i) - t_{i+1,1}(a_{i+1}, b_{i+1}, c_{i+1}) = 0 \quad , \quad i = 1,2,3,4$$

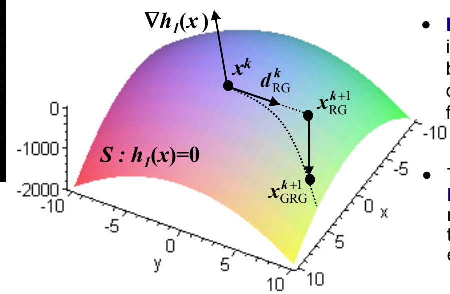
that is:

$$h_i(x) = a_i \cos\left(\frac{2\pi}{365} 365 - b_i \right) + c_i - a_{i+1} \cos\left(\frac{2\pi}{365} - b_{i+1} \right) - c_{i+1} = 0$$

$$i = 1,2,3,4$$

which are nonlinear w.r.t. the decision variables b_i

Generalized Reduced Gradient



- **Problem** : the iterate x^{k+1}_{RG} found by the RG method does not lie on the feasible surface S
- The **Generalized Reduced Gradient** method **(GRG)** tries to keep feasibility at each iterated point.
- The GRG method finds the **new feasible point x^{k+1}_{GRG}, solving numerically (Newton-Raphson)**, at each iteration, the nonlinear system of equations $h(x)=0$, starting at x^{k+1}_{RG} .

Generally Constrained NOP:

Augmented Lagrangian Methods (I)

- Consider, for simplicity, the (GCNOP) with only equality constraints : (GCNOP) $\min_{x} \{ f(x) \mid h(x) = 0 \}$
- The **Augmented Lagrangian** function is defined as :

$$L_A(x, \lambda; c) = f(x) + \lambda^T h(x) + \frac{c}{2} \| h(x) \|^2$$

This Augmented Lagrangian is formed with :

- the Lagrangian function $L(x, \lambda) = f(x) + \lambda^T h(x)$, plus
- the quadratic term $(c/2)\|h(x)\|^2$ that penalizes the infeasibilities of the solution x

($(c/2)\|h(x)\|^2 = 0$ if x is a feasible solution)

Generally Constrained NOP:

Augmented Lagrangian Methods (II)

- The key idea of the Augmented Lagrangian method is to solve the original problem by solving the sequence of **Unconstrained Subproblems**:

$$(\text{US})^k \quad \min_{x} L_A(x, \lambda^k; c^k)$$

, with an increasing sequence $\{c^k\}$, in such a way that **the sequence $\{x^k, \lambda^k\}$ converges to** $\{x^*, \lambda^*\}$ a solution that satisfies the KKT conditions of the original problem.

Generally Constrained NOP:

Augmented Lagrangian Methods (III)

- Note that, for a sufficiently large c^k, the penalty term will dominate in the minimization of $(\text{US})^k$, and then $L_A(x^k, \lambda^k) \approx f(x^k) + \lambda^{k\text{T}} h(x^k)$.
- In this case, the first order optimality conditions of the $(\text{US})^k$ at x^k will be:

$$\nabla L_A(x^k, \lambda^k; c^k) \approx \nabla f(x^k) + \lambda^{k^T} \nabla h(x^k)$$

which are nothing but the KKT conditions for the original problem.

Generally Constrained NOP:

Augmented Lagrangian Methods (III)

- **Framework of the Augmented Lagrangian algorithm**

Given c^0 and starting points x^0 and λ^0, $k:=0$

Do Until (x^k, λ^k) satisfies the KKT conditions.

Compute the new iterate as $x^{k+1} := \operatorname{argmin} L_A(x, \lambda^k, c^k)$

Update the Lagrange multipliers to obtain λ^{k+1}

Choose new penalty parameter $c^{k+1} \geq c^k$

$k:=k+1$

End Do

Generally Constrained NOP:

Projected Lagrangian Methods (I)

- Consider, again, the (GCNOP) with only equality constraints : (GCNOP) $\min_{x}\{f(x) \mid h(x)=0\}$
- **Projected Lagrangian** methods solve the original problem by solving the sequence of **Linearly Constrained Subproblems**:

$$(\text{LCS})^k \begin{cases} \min_x & L_P(x,\lambda^k;c^k) \\ \text{subj. to:} & \nabla h(x^k)(x-x^k)+h(x^k)=0 \end{cases}$$

where the linear constraints comes from the Taylor's series expansion of $h(x)$ around a given point x^k.

Generally Constrained NOP:

Projected Lagrangian Methods (II)

- The most effective expression of the objective function of subproblems (LCS)^k is the **Modified Augmented Lagrangian**:

$$L_P^k(x;\lambda^k,x^k,c)=f(x)+\lambda^{k^T}h^k(x)+\frac{c}{2}\left\|h^k(x)\right\|^2$$

that resembles the Augmented Lagrangian function, excepts that the expression of the nonlinear constraints $h(x)$ has been substituted by $h^k(x)$, defined as:

$$h^k(x)=h(x)-\underbrace{\left[\nabla h(x^k)(x-x^k)+h(x^k)\right]}_{\text{Linear approximation of } h(x) \text{ around } x^k}$$

- Near the solution ($(x^k, \lambda^k) \approx (x^*, \lambda^*)$) the method presents quadratic order of convergence if c=0.

Generally Constrained NOP:

Projected Lagrangian Methods (III)

- **Projected Lagrangian algorithm**

Given c^0 and starting points x^0 and λ^0, $k:=0$

Do Until (x^k, λ^k) satisfies the KKT conditions.

  Solve (LCS)^k to obtain x^{k+1}

  Take λ^{k+1} as the Lag. mult. at the opt. sol. of (LCS)^k

  If $(x^k, \lambda^k) \approx (x^*, \lambda^*)$ **then** set $c^{k+1} = 0$

  Else choose $c^{k+1} \geq c^k$

  $k:=k+1$

End Do

Generally Constrained NOP:

Sequential Quadratic Programming (I)

- Consider, the problem : (GCNOP) $\min_{x}\{f(x) \mid h(x)=0\}$
- **Sequential Quadratic Programming** solves the original problem by solving the sequence of **Quadratic Linearly Constrained Subproblems**:

$$(\text{QLCS})^k \begin{cases} \min_x & \frac{1}{2}(x-x^k)^T W^k (x-x^k)+\nabla f(x^k)(x-x^k) \\ \text{subj. to:} & \nabla h(x^k)(x-x^k)+h(x^k)=0 \end{cases}$$

where the matrix $W^k \in \Re^{n \times n}$ denotes the **Hessian of the Lagrangian function** at (x^k, λ^k) :

$$W^k=\nabla^2_{xx}L(x^k,\lambda^k)=\nabla^2 f(x^k)+\sum_{j=1}^{m}\lambda_j^k\nabla^2 h(x^k)$$

Generally Constrained NOP:

Sequential Quadratic Programming (II)

- **Framework of the Sequential Quadratic Programming**

Given starting points x^0 and λ^0, $k:=0$

Do Until (x^k , λ^k) satisfies the KKT conditions.

Solve (QLCS) ^{k} to obtain x^{k+1}.

Take λ^{k+1} as the Lag. mult. at the opt. sol. of (QLCS) ^{k}

$k:=k+1$

End Do

Generally Constrained NOP:

SQP and Projected Lagrangian

- The strategy of the **SQP** is similar to the one used in the **Projected Lagrangian** methods:
  - **Advantages of SQP**: it is easier to optimize the quadratic subproblem (QLCS)^k than the general (LCS)^k, due to the existence of specialised quadratic programming techniques.
  - **Disadvantages of SQP**: the computation of the quadratic objective function needs the second derivatives (or its numerical approximation) of the objective function $f(x)$ and constraints $h(x)$.
- Both methods can be proved to converge quadratically near the solution.

Solvers for Nonlinear Optimization

Solvers for nonlinear optimization

- **Optimization libraries.**
  - Solving the SIDS problem with the NAG Library
    - Without smoothness constraints.
    - With smoothness constraints.
- **Modeling languages.**
  - Maximization of the constrained likelihood function with AMPL

Optimization libraries:

Description

- Optimization libraries provides subroutines that can be called from the user's own code (mainly in FORTRAN, C or MATLAB).
- In order to solve a problem with an optimization library, the user must provide:
  - The **data structure** with the relevant information about the problem (matrix A in the (LCNOP), lower and upper bounds, etc.)
  - **Subroutines** that, **given a vector** x^k, **returns** all the information needed by the algorithm. This information could be:
    - **At least** $f(x^k)$ and the constraints value $h(x^k)$ and $g(x^k)$.
    - **Usually** the gradients $\nabla f(x^k)$ and Jacobians $\nabla h(x^k)$ and $\nabla g(x^k)$.
    - **Rarely**, the Hessians $\nabla^2 f(x^k)$, $\nabla^2 h(x^k)$ and $\nabla^2 g(x^k)$.

Optimization libraries:

Optimization libraries

- Some of most outstanding optimization libraries are:
  - For Unconstrained Optimization:
    - The optimization subroutines in the NAG and **HARWELL** libraries.
  - For Constrained Optimization:
    - **GRG**, **CONOP**: Generalized Reduced Gradient.
    - **LANCELOT** : Augmented Lagrangians.
    - **MINOS** : Projected Lagrangians.
    - **SNOPT**: Sequential Quadratic Programming.
- But, if you really are interested in knowing all the available optimization software, visit the *NEOS Guide* at www-fp.mcs.anl.gov/otc/Guide/ (a really impressive site in optimization!!)

Optimization libraries:

Solving the SIDS problem with the NAG libraries

- Subroutines for the unconstrained SIDS problem :
  - E04JAF : **Quasi-Newton**, using function values only.
  - E04GCF: **Gauss-Newton**, using function values and first derivatives.
- Subroutines for the constrained SIDS problem:
  - E04UCF: **Sequential Quadratic Programming**, using function values and first derivatives.
- We will see how to solve the SIDS problem calling these subroutines from MATLAB.

Optimization libraries:

Subroutine E04JAF (QN method)

- **Main program**: file SIDS_e04jaf.m

```
% Solving the SIDS problem with the NAG Foundation Library
% Routine E04jaf : Quasi-Newton method using function values only

'Example program for the NAG Foundation Library Routine e04jaf'
SIDS_t;                  % Here the observed data t_{ij} is loaded
x=zeros(15,1);           % Initial point
time=cputime;            % To know the total execution time.
[xQN,f] = e04jaf(x);     % This is the call to the subroutine
Optimal_Objective_Function=f % We print f(x*)...
At_the_Point_X=xQN           % ... the optimal solution x*...
time = cputime-time          % ... and the execution time
```


Optimization libraries:

Subroutine E04JAF (QN method)

- **User's subroutines**: computation of $f(x^k)$ file funct1.m

```
% Objective function for the SIDS problem
function [fc] = funct1(n,xc)
global obs;
fc=0;
ww=(2*pi)/365;
for i=0:4
   aux = 3*i;
   a = xc(1+aux);
   b = xc(2+aux);
   c = xc(3+aux);
   aux2 = 365*i;
    for j=1:365
      calc=a*cos(ww*j-b)+c;
      fc=fc+(calc-obs(j+aux2))^2;
   end
end
fc=fc/2;
```


Optimization libraries:

Subroutine E04JAF (QN method)

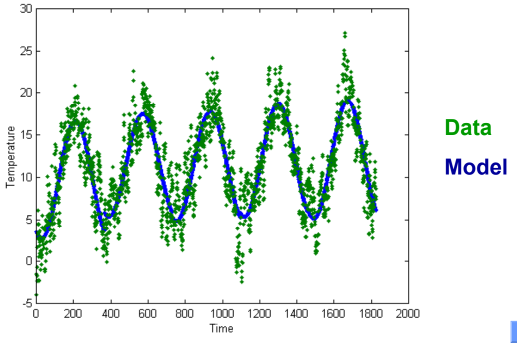
- **Output:**

```
» sids_e04jafe

ans =

Example program for the NAG
Foundation Library Routine
e04jaf


Optimal_Objective_Function =

  6.8569e+003
```

```
At_the_Point_X =
   -6.9691
    0.4920
    9.7255
   -6.0992
    6.7046
   11.4230
   -6.4842
    0.3844
   11.2986
   -6.7013
   -5.8949
   12.0551
   -6.9693
    6.8088
   12.0827

time =
   18.8900
```

Optimization libraries:
Subroutine E04JAF (QN method)

- **Graphical representation :**



Optimization libraries:
Subroutine E04GCF (GN method)

- **Main program**: file SIDS_e04gcf.m

```
% Solving the SIDS problem with the NAG Foundation Library
% Routine E04gcf : Gauss-Newton method using function values
% and first derivatives.

'Example program for NAG Foundation Library routine e04gcf'

SIDS_t;             % Here the observed data t_{ij} is loaded
x = zeros(15,1);    % Initial point
m=length(obs);      % Number of observations
time = cputime;     % To know the total execution time.
[xGN,fsumsq,ifail] = e04gcf(m,x);  % Call to the routine
The_Sum_of_Squares=fsumsq     % We print f(x*)...
At_the_Point_X=xGN            % ... the optimal solution x*...
time = cputime-time           % ... and the execution time
```


Optimization libraries:
Subroutine E04GCF (GN method)

- **User's subroutines**: file lsfun2.m

```
%
% Residuals and its derivatives for the
SIDS problem.
%
% Input :
%
% m           : number of observations.
% n           : number of coefficients.
% xc (n)      : coefficients.
% ljc         : num. Of rows of the Jac..
%
% Output:
%
% fvecc (m)      : vector of residuals.
% fjacc (ljc,n) : Jacobian of the vector
of residual.
%
```

- The output is similar to the previous routine.

graph

```
function [fvecc,fjacc] = lsfun1(m,n,xc,ljc)
global obs;

ww=(2.*pi)/365.;
for i=0:4
   aux = 3*i;
   i_a = aux + 1;
   i_b = aux + 2;
   i_c = aux + 3;
   a = xc(i_a);
   b = xc(i_b);
   c = xc(i_c);
   aux2 = 365*i;
   for j=1:365
     k = aux2 + j;
     calc  = a*cos(ww*j-b)+c;
     fvecc( k) = calc-obs(k);
     fjacc( k, i_a) = cos(ww*j-b);
     fjacc( k, i_b) = a*sin(ww*j-b);
     fjacc( k, i_c) = 1;
   end
end
```

$r_j(x^k)$

$\left.\frac{\partial r_j(x)}{\partial x_i}\right|_{x^k}$

Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Main program**: file SIDS_e04ucf.m

```
% Solving the constrained SIDS problem with the NAG Foundation Library
% Routine E04ucf : SQP method using function values and first derivatives.

'Example program for the NAG Foundation Library Routine e04ucf'
sids_t;           % Loading the observed data
n=15;             % Number of variables.
nclin=0;          % Number of linear constraints.
ncnln=4;          % Number of nonlinear constraints.
a=ones(nclin,1); % Coefficient matrix A (dummy).
bl=-ones(19,1)*1.0E+25; % Default lower bounds for variables and constraints.
bu= ones(19,1)*1.0E+25; % Default upper bounds for variables and constraints.
bl(16:19) = zeros(4,1); % Lower bound for each constraint.
bu(16:19) = zeros(4,1); % Upper bound for each constraint.
x=zeros(15,1);          % Initial point.
confun='SIDS_e04ucf_confune'; % User's subroutine for the constraints and Jacobian.
objfun='SIDS_e04ucf_objfune'; % User's subroutine for the o.f. and gradient.
```

Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Main program**: file SIDS_e04ucf.m (cont.)

```
% Optimization parameters:
    string = ' Infinite Bound Size = 1.0e25 ';
    e04uef(string);
    string = ' Print Level = 1 ';
    e04uef(string);
    string = ' Verify Level = -1 ';
    e04uef(string);
% Call to the optimizer:
    [iter,c,objf,objgrd,x,cjac,istate,clamda,r,ifail] = ...
    e04ucf(bl,bu,confun,objfun,x,ncnln,a);
```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Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **User's subroutines**: computation of $f(x^k)$ and $\nabla f(x^k)$: file SIDS_e04ucf_objfune.m

```
%
% Function "objfun" for the constrained SIDS problem
%
% Input:
%
% mode      : information required
% n         : number of variables
% x (n)     : current iterate x^k
% nstate    : information about the current iterate
%
% Output
%
% objf       : objective function at x^k.
% objgrd (n) : gradient vector at x^k
%
 function [mode,objf,objgrd] = objfun(mode,n,x,objf,objgrd,nstate)
```


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Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **User's subroutines**: computation of $f(x^k)$ and $\nabla f(x^k)$: file SIDS_e04ucf_objfune.m

```
function [mode,objf,objgrd] = objfun(mode,n,x,objf,objgrd,nstate)
%
global obs;
ww=(2*pi)/365;
%
if mode==0 | mode==2 % Evaluation of f(x^k)
  F=0;
  for i=0:4
    aux = 3*i;
    a = x(1+aux);
    b = x(2+aux);
    c = x(3+aux);
    aux2 = 365*i;
    for j=1:365
        res = a*cos(ww*j-b)+c - obs(j+aux2);
        F=F+res^2;
    end
  end
  objf=F/2;
end
```


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Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **User's subroutines**: computation of $f(x^k)$ and $\nabla f(x^k)$: file SIDS_e04ucf_objfune.m

```
if mode==1 | mode==2 % Evaluation of the gradient
  G=zeros(1,15);
  for i=0:4
    aux1 = 3*i;
    i_a = 1 + aux1;
    i_b = 2 + aux1;
    i_c = 3 + aux1;
    a = x(i_a);
    b = x(i_b);
    c = x(i_c);
    aux2 = i*365;
    for j=1:365
      res = a*cos(ww*j-b)+c - obs(j+aux2);
      G(i_a)=G(i_a)+res*cos(ww*j-b) ;
      G(i_b)=G(i_b)+res*sin(ww*j-b);
      G(i_c)=G(i_c)+res;
    end
    G(i_b) = a*G(i_b);
  end
end
objgrd = G;
```

Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **User's subroutines**: computation of $h(x^k)$ and $\nabla h(x^k)$: file SIDS_e04ucf_confune.m

```
%
% Function "objfun" for the constrained SIDS problem
%
% Input:
%
% mode           : information required
% ncnln          : number of rows of the Jacobian.
% n              : number of variables
% nrows          : max(1,ncnln)
% needc(ncnln)   : flag to indicate the constraints to be evaluated.
% x (n)          : current iterate x^k
% nstate         : information about x^k.
%
% Output
%
% c (ncnln)      : value of the constraints over x^k
% cjac (nrowj,n) : Jacobian over x^k
%
 function [mode,c,cjac] = confun(mode,ncnln,n,nrowj,needc,x,c,cjac,nstate)
%
```


Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **User's subroutines**: computation of $h(x^k)$ and $\nabla h(x^k)$: file SIDS_e04ucf_confune.m

```
if nstate==1
  cjac=zeros(ncnln,n);
end

ww = 2*pi/365;

for i=1:4
   aux = 3*(i-1);
   a0 = x(aux+1);
   b0 = x(aux+2);
   c0 = x(aux+3);
   a1 = x(aux+4);
   b1 = x(aux+5);
   c1 = x(aux+6);
   aux0 = ww*365.;
   aux1 = ww;
   cos0 = cos(aux0 - b0);
   sin0 = sin(aux0 - b0);
   cos1 = cos(aux1 - b1);
   sin1 = sin(aux1 - b1);
    if needc(i)>0
    % Continuity of y(j,t) at the "i"-th connect point
    if mode==0 | mode==2
          c(i) = a0*cos0 + c0 - ( a1*cos1 + c1);
      end
      if mode==1 | mode==2
          cjac(i,aux+1) = cos0;
          cjac(i,aux+2) = a0*sin0;
          cjac(i,aux+3) = 1.;
          cjac(i,aux+4) = -cos1;
          cjac(i,aux+5) = -a1*sin1;
          cjac(i,aux+6) = -1.;
       end
    end
end
```

$$h_i(x) = a_i \cos\left(\frac{2\pi}{365}365 - b_i\right) + c_i - a_{i+1}\cos\left(\frac{2\pi}{365} - b_{i+1}\right) - c_{i+1}$$

$$\left.\frac{\partial h_i(x)}{\partial x_j}\right|_{x^k}$$

Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Output (I):**

```
» sids_e04ucfE

ans =

Example program for the NAG Foundation Library Routine e04ucf



 Calls to E04UEF
 ---------------

       Infinite Bound Size = 1.0e25
       Print Level = 1
       Verify Level = -1

 *** E04UCF
 *** Start of NAG Library implementation details ***

 Implementation title: Microsoft Windows NT Powerstation
            Precision: FORTRAN Double Precision
         Product Code: FLNTI17DI
                 Mark: 17A

 *** End of NAG Library implementation details ***
```


Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Output (II) :**

```
Parameters
 ----------

 Linear constraints.....         0      Variables.............        15
 Nonlinear constraints..         4

 Infinite bound size....  1.00D+25      COLD start.............
 Infinite step size.....  1.00D+25      EPS (machine precision)  1.11D-16
 Step limit.............  2.00D+00      Hessian................        NO

 Linear feasibility.....  1.05D-08      Crash tolerance........  1.00D-02
 Nonlinear feasibility..  1.05D-08      Optimality tolerance...  3.26D-12
 Line search tolerance..  9.00D-01      Function precision.....  4.38D-15

 Derivative level.......         3      Monitoring file........        -1
 Verify level...........        -1

 Major iterations limit.        85      Major print level......         1
 Minor iterations limit.        57      Minor print level......         0

 Workspace provided is     IWORK(      53),  WORK(     954).
 To solve problem we need  IWORK(      53),  WORK(     954).
```

Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Output (III):**

```
Exit from NP problem after    33 major iterations,
                              34 minor iterations.

 Varbl State      Value       Lower Bound   Upper Bound  Lagr Mult   Slack

 V   1   FR   -6.01843          None          None
 V   2   FR    6.86197          None          None
 V   3   FR   10.2776           None          None
 V   4   FR   -6.45854          None          None
 V   5   FR    6.68295          None          None
 V   6   FR   11.2311           None          None
 V   7   FR   -6.46699          None          None
 V   8   FR    6.67074          None          None
 V   9   FR   11.3104           None          None
 V  10   FR   -7.00733          None          None
 V  11   FR    6.65565          None          None
 V  12   FR   11.8928           None          None
 V  13   FR    7.33845          None          None
 V  14   FR    9.92259          None          None
 V  15   FR   11.8731           None          None
```

x^*

Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Output (IV):**

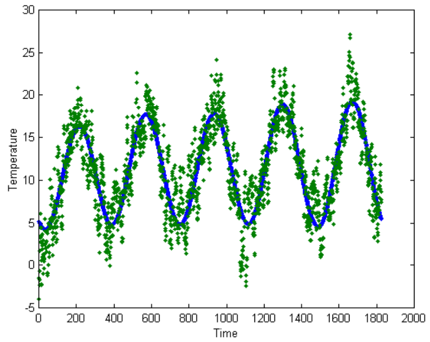
```
N Con State      Value        Lower Bound   Upper Bound   Lagr Mult    Slack

 N   1   EQ   -1.267431E-11       .             .           201.5     1.2674E-11
 N   2   EQ    2.171596E-11       .             .           131.5    -2.1716E-11
 N   3   EQ    7.942980E-12       .             .           135.8    -7.9430E-12
 N   4   EQ   -3.250733E-13       .             .            76.53    3.2507E-13

 Exit E04UCF - Optimal solution found.

 Final objective value =      7082.574
»
```

$h(x^*)$ λ^*

$f(x^*)$

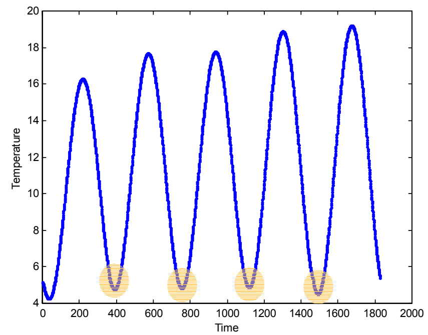
Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Graphical representation of the solution :** data and model



Optimization libraries:
Constrained SIDS with subroutine E04UCF

- **Graphical representation of the solution :** model



Now the model is continuous

Modeling languages: Introduction

- **Modeling languages** can be saw as a friendly interface between the user and the optimization libraries.
- The way this applications work is :
  - The user **defines the optimization problem** to be solved (objective function and constraints) in a notation very similar to the natural mathematical notation.
  - Then, he **selects the solver** to be used (MINOS, LANCELOT, CONOPT, etc).
  - The application **automatically translates the model defined by the user** to the specific input data structure needed by the selected solver.

Modeling languages: Advantages/Disadvantages

- **Advantages:** the developing time is shortened, because
  - The definition of the model is very easy, because the syntax of the modeling language resembles the usual mathematical notation.
  - The model definition is independent of the solver to be used. That means that, after defining just once the optimization problem, the user are able to solve it with a great variety of solvers, forgetting all the annoying issues related with the specific data structure of each solver.
- **Disadvantages:** the execution time increases compared with the one obtained directly using the optimization libraries.
- **Conclusion**: this approach is appropriate:
  - For small scale problems, where the execution time is not critical.
  - To develop prototype implementations to achieve a deeper comprehension of the model, before its implementation in FORTRAN o C.

Modeling languages: GAMS/AMPL

- **Modeling languages** : the two modeling languages most widely used are:
  - **GAMS** (www.gams.com) :
    General Algebraic Modeling System
  - **AMPL** (www.ampl.com) :
    A Modeling Language for Mathematical Programming
- We will use AMPL to illustrate the use of this sort of software, solving the constrained likelihood maximization problem

Modeling languages: A Log-Likelihood Function

(Langohr, Gómez, 1BWSA Poster Session, thursday)

$$
\text{(LCNOP)}\left\{
\begin{aligned}
\max_{\grave{u},\alpha,\beta,\sigma}\quad & l(\grave{u},\alpha,\beta,\sigma)=\sum_{i=1}^{n}\Bigg[\varepsilon_i\xi_{1i}\ln\left(\sum_{j=1}^{m}\frac{\gamma_{ij}}{\sigma}\exp\left[\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}-e^{\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}}\right]\omega_j\right)\\
&\quad+\varepsilon_i\xi_{2i}\ln\left(\sum_{j=1}^{m}\gamma_{ij}\exp\left[-e^{\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}}\right]\omega_j\right)\\
&\quad+\varepsilon_i(1-\xi_{1i})(1-\xi_{2i})\ln\left(\sum_{j=1}^{m}\gamma_{ij}\left(1-\exp\left[-e^{\frac{\ln(y_{obs,i}+z_{obs,i}-s_j)-\alpha-\beta\ln(s_j)}{\sigma}}\right]\right)\omega_j\right)\\
&\quad+(1-\varepsilon_i)\ln\left(\sum_{j=1}^{m}\gamma_{ij}\omega_j\right)\Bigg]\\
\text{subj.to:}\quad & \sum_{j=1}^{m}\omega_j=1\\
& \omega_j\ge 0\quad,\quad j=1,2,\ldots,m\\
& \sigma\ge 0
\end{aligned}
\right.
$$

With α, β, σ, and ω decision variables, and ε, ξ and γ known parameters

Modeling languages:
User's data files with AMPL

- In order to solve the (LCNOP) Log-Likelihood problem with AMPL, the user must first define:
  - A Model file with:
    - The declaration of the decision variables $\omega,\alpha,\beta,\sigma$ and its bounds.
    - The mathematical expressions of the o.f. $l(\omega,\alpha,\beta,\sigma)$
    - The mathematical expression of the linear constraint.
  - A Data file with the definition of all the know parameters of the model (m, n and ε, ξ and γ).
  - A Run file which is a script file, a sort of main program, with the list of commands to be executed to solve the defined problem.
- And then, solve the problem with AMPL

Modeling languages:
The model file for the Log-Likelihood problem

- **Definition of the model:** file 1bwsa.mod

```
# Parameters of the model ##############################
set V;          # set for variables
param Lb{V};    # bounds for variables
param Ub{V};
param M ;       # number of possible covariate values
param N ;       # number of observations
param pi := 3.14159265;
param gamma{1..N,1..M};   # matrix for censoring pattern of covariate
param y{1..N};          # time from HIV+ to observed value for AIDS
param epsi{1..N};       # observation indicator for y
param xi_1{1..N};       # exact observation indicator for y
param xi_2{1..N};       # right-censored observation indicator for y
param hivn{1..N};       # time to HIV: left endpoint
param hivp{1..N};       # time to HIV: right endpoint
param s{1..M};          # values of time till HIV
param logsum{1..N,1..M}; # possible values for log(time from HIV till AIDS)
param RR_zeta;          # relative risk for current status covariate (csc)
param acc_fac_z;        # accelerating factor for csc
```


Modeling languages:
The model file for the Log-Likelihood problem

- **Definition of the model:** file 1bwsa.mod (cont.)

```
# Decision variables ################################
    var alpha;
    var beta;
    var sigma >= 0, :=1;
    var omega{j in 1..M} >=0;
# Objective function #################################
    maximize logLikelihood:
      sum{i in 1..N}
        (epsi[i]*xi_1[i]*log(1/sigma*sum{j in 1..M}
         gamma[i,j]*exp((logsum[i,j]-alpha-beta*log(s[j]))/sigma-
    exp((logsum[i,j]-alpha-beta*log(s[j]))/sigma))*omega[j])+
         epsi[i]*xi_2[i]*log(sum{j in 1..M} gamma[i,j]*exp(-
    exp((logsum[i,j]-alpha-beta*log(s[j]))/sigma))*omega[j])+
         epsi[i]*(1-xi_1[i])*(1-xi_2[i])*log(sum{j in 1..M}
      gamma[i,j]*(1-exp(-exp((logsum[i,j]-alpha-
    beta*log(s[j]))/sigma)))*omega[j])+
        (1-epsi[i])*log(sum{j in 1..M} gamma[i,j]*omega[j]));
# Linear constraint ##################################
    subject to sum1:
       sum {i in 1..M} omega[i] = 1;
```


Modeling languages:
The data file for the Log-Likelihood problem

- **Data:** file 1bwsa.dat

```
set V:= 1,2,3;

param:  Lb  Ub :=
   1    -15   15
   2    -15   15
   3      0   15;

param M := 215;
param N := 361;

param:  hivn  hivp   y    epsi  xi_1  xi_2:=
   1     1     45    36     1     1    0
   2     1     83    36     1     0    1
   3     1     112   1      1     1    0
   4     1     84    9      1     1    0
   5     1     37    76     1     0    1
   ....................................
 359   107     215   9999   0     0    0
 360    83     215   9999   0     0    0
 361     8     215   9999   0     0    0;
```

215+3 = 218 decision variables

Modeling languages:

The script file for the Log-Likelihood problem

- **Execution file :** file 1bwsa.run

```
# First, the model and data are loaded :
    model 1bwsa.mod;
    data 1bwsa.dat;
# Now the fixed parameters of the model are computed :
    for{j in 1..M}{
     let omega[j] := 1/M;
     let s[j] := j;
    }
    for{i in 1..N}{
      for{j in 1..M}{
        if hivn[i] <= s[j] and s[j] <= hivp[i]
        then let gamma[i,j]:= 1;
        else let gamma[i,j]:= 0;
      }
    }
    for{i in 1..N}{
      for{j in 1..M}{
        if gamma[i,j]==1 and epsi[i]==1
        then let logsum[i,j]:= log(y[i]+hivp[i]-s[j]);
        else let logsum[i,j]:= 0;
      }
    }
```


Modeling languages:

The script file for the Log-Likelihood problem

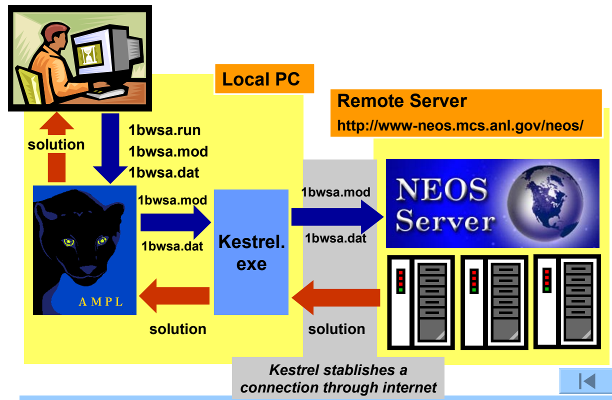
- **Execution file :** file 1bwsa.run (cont.)

```
# Here we choose the optimizer
  option solver kestrel; # remote optimization at the NEOS Server...
  option kestrel_options 'solver=snopt'; #...with the SNOPT optimizer
  option snopt_options "version";
# and now, we solve ...
  solve;
# ...and print the solution :
  let RR_zeta:= exp(-beta/sigma);
  let acc_fac_z:= exp(beta);
  printf "The estimated values of the model are (alpha, beta, sigma)
  = (%6.4f, %6.4f, %6.4f).\n",alpha, beta, sigma;
  printf "The relative risk amounts to %5.4f,", RR_zeta; printf " the
  accelerating factor is %5.4f.\n", acc_fac_z;
  option omit_zero_rows 1;
  display omega;
```

What means "*remote optimization*"?

Modeling languages:

Remote optimization through the NEOS Server



Modeling languages:

Resolution of the Log-Likelihood problem

- **Results :**

Execution command line

```
DOS> ampl 1bwsa.run
```

Tracking information of the remote server

```
Job has been submitted to Kestrel
Kestrel/NEOS Job number    : 163559
Kestrel/NEOS Job password  : irQEgUIl
Check the following URL for progress report :
     http://www-neos.mcs.anl.gov/neos/neos-cgi/check-
status.cgi?job=163559&pass=irQEgUIl
In case of problems, e-mail :
     neos-comments@mcs.anl.gov
```

Information about the remote optimization process

```
Intermediate Solver Output:
Checking the AMPL files
Executing algorithm...
SNOPT 6.1-1(5)(Nov 2001): version
Finished call
```

Modeling languages:

Resolution of the Log-Likelihood problem

- **Results : (cont.)**

Information sent by the remote optimization server

```
SNOPT 6.1-1(5)(Nov 2001):
Optimal solution found.
1882 iterations, objective -444.6446856
Nonlin evals: obj = 201, grad = 200.
```

Solution printed by the local 1bwsa.run file

```
The estimated values of the model are (alpha, beta, sigma) =
(4.8218, 0.1374, 0.4752).
The relative risk amounts to 0.7490, the accelerating factor
is 1.1472.
omega [*] :=
  1  0.0407
  6  0.156988
 10  0.0827764
 24  0.167377
 36  0.0762982
 48  0.126317
 59  0.0737118
 60  0.0258302
 83  0.0796388
 95  0.0172243
119  0.073086
202  0.0800525
```

Only the nonzero variables ω_j are shown