$$f(x) = 4x_1^2 + 2x_1x_2 + 5x_2^2 + x_1 + 3x_2$$

1) Write the Taylor expansion at $\begin{pmatrix}0\\0\end{pmatrix}$ of order 2

$$f(x) = f\begin{pmatrix}0\\0\end{pmatrix} + \langle \nabla f\left(\begin{pmatrix}0\\0\end{pmatrix}\right), x\rangle + \frac{1}{2}\langle Hf\begin{pmatrix}0\\0\end{pmatrix}x, x\rangle + o(\|x\|^2)$$

$$\nabla f(x) = \begin{pmatrix} 8x_1 + 2x_2 + 1 \\ 2x_1 + 10x_2 + 3 \end{pmatrix} \qquad Hf(x) = \begin{pmatrix} 8 & 2 \\ 2 & 10 \end{pmatrix}$$

$$\det(Hf(x) - \lambda I) = (8-\lambda)(10-\lambda) - 4 = \lambda^2 - 18\lambda - 4$$

$$\Delta = 18^2 - 16 > 0$$

$$\lambda_i = \frac{18 \pm \sqrt{\Delta}}{2} > 0$$

$$\nabla f\begin{pmatrix}0\\0\end{pmatrix} = \begin{pmatrix}1\\3\end{pmatrix} \qquad Hf\begin{pmatrix}0\\0\end{pmatrix} = \begin{pmatrix} 8 & 2 \\ 2 & 10 \end{pmatrix}$$

$$f(x) = 0 + \langle \begin{pmatrix}1\\3\end{pmatrix}, x\rangle + \frac{1}{2}\langle Hf(0)x, x\rangle + ?\ \boxed{0}$$

because $Hf(x) = cte$

$$= \frac{1}{2}\langle Ax, x\rangle + \langle b, x\rangle + c \qquad A \in S^n_{++}$$

$$A = Hf\begin{pmatrix}0\\0\end{pmatrix} \qquad b = \nabla f\begin{pmatrix}0\\0\end{pmatrix} \qquad c = f\begin{pmatrix}0\\0\end{pmatrix}$$

$$f(x^*) = \min f(x) \iff \nabla f(x^*) = 0 \iff \quad x^* = ?$$

Conjugate gradient method : motivation

has been developped for quadratic functions in high dimension : $f(x) = \frac{1}{2}\langle Ax, x\rangle + \langle b, x\rangle + c$

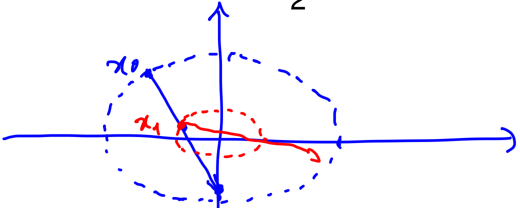
$A \in S^n_{++}$ $\quad b \in \mathbb{R}^n$

$$
\begin{aligned}
f(x^*) &= \inf_{x \in \mathbb{R}^n} f(x) \\
f(x) &= \frac{1}{2}(\alpha_1 x_1^2 + \alpha_2 x^2), \quad \text{with } 0 < \alpha_1 < \alpha_2 \\
&= \frac{1}{2}\langle Ax, x\rangle \quad \text{with } A = \begin{pmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix}
\end{aligned}
$$

$\alpha_1 = 1 \quad \alpha_2 = 2$

$\nabla f(x) = \begin{pmatrix} \alpha_1 x_1 \\ \alpha_2 x_2 \end{pmatrix}$

$\nabla f\begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \end{pmatrix}$



$x_1 = x_0 - \alpha_0 \nabla f(x_0)$

$x_k \xrightarrow[k \to \infty]{} x^* = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

but $x_k \neq x^*$ $\forall k$

there is a better choice than $-\nabla f(x)$ for the descent

A-conjugate directions

$f(x) = \frac{1}{2}\langle Ax, x\rangle + \langle b, x\rangle$

Definition : Let $A \in S^n_{++}$.

- 2 non zero vectors v, w are called $A-$conjugate iff $\langle Av, w\rangle = 0$. $= \langle v, Aw\rangle$
- A family of non zero vectors $(v_i)_{i=1,\dots m}$, is called $A-$conjugate iff $\langle Av_i, v_j\rangle = 0$ for all $i = 1, \dots, m$, $j = 1, \dots, m$, $i \neq j$.

Property : $A-$conjugate vectors are linearly independent. If $m = n$ a $A-$conjugate family is a basis of $\mathbb{R}^n$.

Definition : a conjugate descent method is a method where the successive descent directions form a $A-$conjugate family

Expression of the minimum of f in a $A-$conjugate basis

the minimum of $f(x)$ satisfies $\nabla f(x^*)=0$
$Ax^*+b=0$

$$f(x) = \frac{1}{2}\langle Ax, x\rangle + \langle b, x\rangle$$

Suppose we have a basis $(d_i)_{i=1,\dots,n}$, such that $\langle Ad_i, d_j\rangle = 0$ for $j \neq i$

$$x^\star = \sum_{i=1}^{n} \alpha_i d_i, \text{ and } Ax^\star + b = 0,$$

$$\text{therefore } Ax^\star = -b = \sum_{i=1}^{n} \alpha_i A d_i, \text{ then for any } j = 1, \dots, n$$

$$-\langle b, d_j\rangle = \sum_{i=1}^{n} \alpha_i \langle Ad_i, d_j\rangle = \alpha_j \langle Ad_j, d_j\rangle$$

$$\alpha_j = \frac{-\langle b, d_j\rangle}{\langle Ad_j, d_j\rangle}$$

Construction of the $A-$conjugate basis iteratively

choose initial point x_0 $\quad g_0 = Ax_0 + b$

Let $g_k = \nabla f(x_k) = Ax_k + b$ be the gradient at step k
Choose $d_0 = -g_0$ (The first step is a standard gradient descent step)
Then $d_k = -g_k + \beta_{k-1} d_{k-1}$ satisfying: $\quad \beta_{k-1} \in \mathbb{R}$
(CG1) $\quad \langle Ad_k, d_j \rangle = 0$ for $j = 0, \ldots, k-1$ and
(CG2) $\quad \langle g_k, d_j \rangle = 0$ for $j = 0, \ldots, k-1$

$d_1 = -g_1 + \beta_0 d_0$
$\langle Ad_1, d_0 \rangle = 0$
$\langle g_1, d_0 \rangle = 0$

Update at step k : $x_{k+1} = x_k + \alpha_k d_k$
Next gradient $g_{k+1} = Ax_{k+1} + b = g_k + \alpha_k Ad_k$
Property : For all initial guess x_0 there exists $(\alpha_k)_k$ and $(\beta_k)_k$ such that (CG1) and (CG2) are satisfied.
Property : (CG1) and (CG2) $\Rightarrow \langle g_k, g_j \rangle = 0$ for $j \neq k$

$Ax_1 + b = g_0 + \alpha_0 Ad_0$
$\langle g_1, d_0 \rangle = 0 = \langle g_0, d_0 \rangle + \alpha_0 \langle Ad_0, d_0 \rangle = 0 \quad \longrightarrow \quad \alpha_0 = \dfrac{-\langle g_0, d_0 \rangle}{\langle Ad_0, d_0 \rangle}$

Convergence of a conjugate method

Property : A conjugate descent method using directions satisfying conditions (CG1) and (CG2) converges in at most n steps.

Property : $\beta_k = -\frac{\langle Ad_{k-1}, g_k \rangle}{\langle Ad_{k-1}, d_{k-1} \rangle} = \frac{\|g_k\|^2}{\|g_{k-1}\|^2}$.

$d_k = -g_k + \beta_{k-1} d_{k-1}$

Property : $\alpha_k = -\frac{\langle g^k, d^k \rangle}{\langle Ad^k, d^k \rangle}$

$x_{k+1} = x_k + \alpha_k d_k$

Conjugate gradient algorithm

Data: Matrix A, vector b, tolerance ε
Result: $x^\star$ such that $f(x^\star) = \min_x f(x)$
Initialisation : $k = 0$,
Initial guess for solution $x^0 \in \mathbb{R}^n$
$g^0 = Ax^0 + b$
$d^0 = -g^0$
while $\|g^k\| > \varepsilon$ **do**

- Compute directionnal minimum :
  $v^k = Ad^k$
  $\alpha_k = -\dfrac{\langle g^k, d^k\rangle}{\langle v^k, d^k\rangle}$
  $x^{k+1} = x^k + \alpha_k d^k$
- Update gradient :
  $g^{k+1} = g^k + \alpha_k v^k$
- Compute new direction :
  $\beta_{k+1} = \dfrac{\langle g^{k+1}, g^{k+1}\rangle}{\langle g^k, g^k\rangle}$
  $d^{k+1} = -g^{k+1} + \beta_{k+1} d^k$

$k \leftarrow k + 1$

same as the standard gradient descent method with optimal step

2

end
$x^\star \leftarrow x^k$

Monotonicity of the conjugate gradient algorithm

Property : If $d_k \neq 0$ and $\alpha_{k+1} \neq 0$ then $f(x_{k+1}) < f(x_k)$.
If $\alpha_{k+1} = 0$, x_k is the minimizer of f and $Ax_k + b = 0$

Polak-Ribière method

for non quadratic $f : \mathbb{R}^n \to \mathbb{R}$

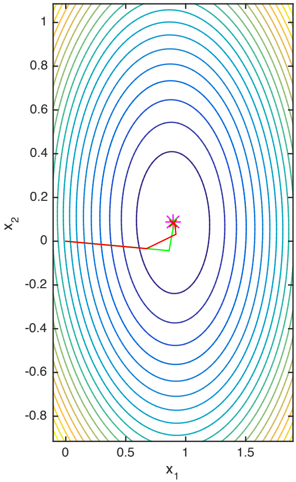
Data: Function f, gradient ∇f, tolerance ε
Result: $x^\star$ such that $f(x^\star) = \min_x f(x)$
Initialisation : $k = 0$,
Initial guess for $x^0 \in \mathbb{R}^n$
$g^0 = \nabla f(x^0)$
$d^0 = -g^0$
while $\|g^k\| > \varepsilon$ *and* $k < k_{\max}$ **do**

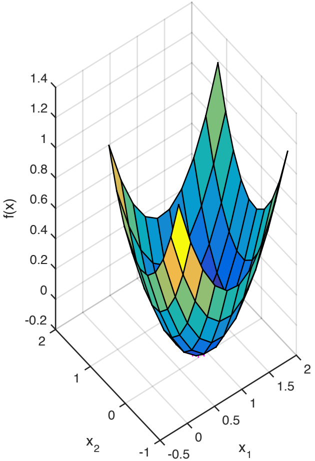
- Compute ~~the step in direction d_k~~: an admissible step in the direction
  $f(x^k + \alpha_k d^k) \cancel{\leq f(x^k + \alpha d^k)} < f(x^k)$ ~~for all $0 < \alpha \leq \alpha_k$~~
- Compute new position :
  $x^{k+1} = x^k + \alpha_k d^k$
- Compute new direction :
  $g^{k+1} = \nabla f(x^{k+1})$
  $c_{k+1} = \dfrac{\langle g^{k+1} - g^k, g^{k+1} \rangle}{\langle g^k, g^k \rangle}$
  $d^{k+1} = -g^{k+1} + c_{k+1} d^k$

$k \leftarrow k + 1$
end
$x^\star \leftarrow x^k$

Comparaison of conjugate Gradient (green, 4 steps)and Polak-Ribière (red, 8 steps) methods.

f quadratic function in $\mathbb{R}^5$. Projection on $(0, x_1, x_2)$.





Linear regression

$m >> n$ if at least n points are different $rg(X) = n$

Find θ defining a linear model $\theta \in \mathbb{R}^n$ $\quad h_\theta : \mathbb{R}^n \to \mathbb{R}$

$$\hat{y} = h_\theta(x) = \theta^T.x$$

Let m measurements (x_i, y_i), $i = 1, \ldots, m$, where explaining variables are in $\mathbb{R}^n$ $(x_i = (x_i^j)_{j=1,\ldots,n}$. θ is found by minimizing the least squared error

$$Y = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}$$

$$E(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(\theta^T.x_i - y_i\right)^2. = \frac{1}{m}\|X\theta - Y\|^2$$

$$X = \begin{pmatrix} x_1^1 & \cdots & x_1^n \\ \vdots & & \\ x_m^1 & \cdots & x_m^n \end{pmatrix}$$

The normal equation gives the best solution

$f(\theta) = \|X\theta - Y\|^2$

$\nabla f(\theta) = 2X^T(X\theta - Y)$

$\nabla f(\hat{\theta}) = 0$

$$\hat{\theta} = (X^T.X)^{-1}.X^T.y$$

complexity in $O(n^3)$ and $O(m)$.

Outline

Nonlinear least squares

$$f : \begin{cases} \mathbb{R}^P & \rightarrow & \mathbb{R}^Q \\ x = (x_1, \ldots, x_P)^t & \mapsto & (f_1(x), \ldots, f_Q(x))^t \end{cases}$$

for $Q > P$ we seek a solution to the problem $f(x) = 0$.

even if $Q = P$ $f(x) = 0$ is difficult

$\Downarrow$

Newton

Examples

- Find a line that passes through Q points with $Q > 2$

if the points are not aligned the Pb has no solution

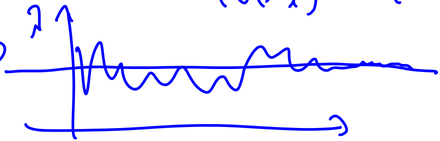
$g(x) = \|f(x)\|^2$ minimise $g(x)$

Examples

- Find the parameters N_0 and λ of a radioactive material whose emissions are monitored over time $N(t) = N_0 e^{-\lambda t}$

each month you measure $N(t_i) = N_i$

$$\min_{N_0,\lambda} \sum_{i=1}^{m} \| N_0 e^{-\lambda t_i} - N_i \|^2 \longrightarrow$$



Toy example

Q is the number of months were you measured N_i

$N_0 = x_1 \quad \lambda = x_2$

Q measurements $N_i \sim N(t_i) = N_0 e^{-\lambda t_i} \quad i = 1, \dots, Q$

$f : \mathbb{R}^2 \to R^Q$ with Q large

$(N_i)_{i=1,\dots,Q}$ radioactivity measurements at times $(t_i)_{i=1,\dots,Q}$

$$f(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_Q(x) \end{pmatrix} = \begin{pmatrix} x_1 e^{-x_2 t_1} - N_1 \\ x_1 e^{-x_2 t_2} - N_2 \\ \vdots \\ x_1 e^{-x_2 t_Q} - N_Q \end{pmatrix}.$$

$f(x) = 0$

Calculate the Jacobian matrix $Jf(x)$

Toy example

$f : \mathbb{R}^2 \to R^Q$ with Q large

$(N_i)_{i=1,\dots,Q}$ radioactivity measurements at times $(t_i)_{i=1,\dots,Q}$

$$f(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_Q(x) \end{pmatrix} = \begin{pmatrix} x_1 e^{-x_2 t_1} - N_1 \\ x_1 e^{-x_2 t_2} - N_2 \\ \vdots \\ x_1 e^{-x_2 t_Q} - N_Q \end{pmatrix}.$$

Calculate the Jacobian matrix $Jf(x)$

$$Jf(x) = \begin{pmatrix} e^{-x_2 t_1} & -x_1 t_1 e^{-x_2 t_1} \\ e^{-x_2 t_2} & -x_1 t_2 e^{-x_2 t_2} \\ \vdots & \\ e^{-x_2 t_Q} & -x_1 t_Q e^{-x_2 t_Q} \end{pmatrix}.$$

Reminders: linear least squares

$Ax = b$ for $b \in \mathbb{R}^Q$ and $A \in \mathcal{M}_{Q,P}(\mathbb{R})$ with $Q > P$ and $\mathrm{rg}(A) = P$.
The problem: find $x \in \mathbb{R}^P$ such that

$$\|Ax - b\|^2 = \min_{y \in \mathbb{R}^P} \|Ay - b\|^2$$

admits a unique solution given by the normal equation

$$A^t A x = A^t b.$$

Nonlinear case

instead of looking for $f(x^*) = 0$ (which doesn't not exists)

we minimize $g(x) = \|f(x)\|^2 = \sum_{i=1}^{Q} f_i(x)^2$

$$g(x^*) = \begin{cases} \text{Find } x^* \in \mathbb{R}^P \text{ such that} \\ \|f(x^*)\|^2 = \min_{x \in \mathbb{R}^P} \|f(x)\|^2 \quad \left(\|f(x)\|^2 = \sum_{k=1}^{Q} (f_k(x))^2 \right), \end{cases}$$

We suppose that :

$$\forall x \in \mathbb{R}^P, \qquad J_f(x) \in \mathcal{M}_{Q,P}(\mathbb{R}) \text{ has rank } P.$$

In particular, we will have $(J_f(x))^t J_f(x)$ symmetric defined positive.

Nonlinear case (continued)

$f : \mathbb{R}^2 \to \mathbb{R}^Q$ $\quad z \in \mathbb{R}^2$

$g(x) = \|f(x)\|^2 = N \circ f$ with $N(y) = \|y\|^2$

$Dg(x)h = DN(f(x))\, Df(x)h$

$= \langle 2f(x), Jf(x)h \rangle$

$DN(y)h = \langle 2y, h \rangle$

$Df(x)z = Jf(x)z$

We notice

$$g : \begin{cases} \mathbb{R}^P & \to & \mathbb{R} \\ x & \mapsto & \|f(x)\|^2 \end{cases}$$

If g is strictly convex and coercive then the problem $g(x^*) = \min_x g(x)$ admits a unique solution x^*

$$\nabla g(x^*) = 0.$$

$Dg(x)h = \langle 2\, Jf(x)^T f(x), h \rangle$

$\nabla g(x) = 2\, Jf(x)^T f(x)$

$Jf(x) \in \mathcal{M}_{Q \times 2}(\mathbb{R})$

Calculating the gradient of g

$g = Nof$ composition of
$N : \mathbb{R}^Q \to \mathbb{R}$, $N(y) = ||y||^2$ and $f : \mathbb{R}^P \to \mathbb{R}^Q$.
The rule for differentiating a composite function gives
$Dg(x) = DN(f(x))Df(x)$
For $y, \delta \in \mathbb{R}^Q$, $DN(y)\delta = \langle 2y, \delta\rangle$
for $x, h \in \mathbb{R}^P$, $Df(x)h = Jf(x)h \in \mathbb{R}^Q$

$$h, x \in \mathbb{R}^P, \quad Dg(x)h = \langle 2f(x), Jf(x)h\rangle = \langle 2Jf(x)^T f(x), h\rangle$$

$$\nabla g(x) = 2Jf(x)^T f(x).$$

Find the zeros of ∇g or the zeros of $f(x)$

$P=2$ for our example

- $\boxed{\nabla g(x) = 2Jf(x)^T f(x)}$ Newton method requires $Hf(x)$
- If $f(x)$ is a function of $\mathbb{R}^P$ in $\mathbb{R}^P$ we find the zeros by Newton's algorithm

$$x_{k+1} = x_k + d_k$$

$$\text{with } Jf(x_k)d_k = -f(x_k).$$

- Here $f(x)$ is a function of $\mathbb{R}^P$ in $\mathbb{R}^Q$ so the system $\boxed{Jf(x_k)d_k = -f(x_k) \text{ of size } Q \times P}$ is solved in the least squares sense

given the best solution for $f(x_k)=0$

$$\boxed{Jf(x_k)^T Jf(x_k)d_k = -Jf(x_k)^T f(x_k)}$$

$$\Leftrightarrow \quad d_k = -(Jf(x_k)^T Jf(x_k))^{-1} Jf(x_k)^T f(x_k).$$

Gauss Newton method for N.L. systems of equations

- Initialize $x_0 \in \mathbb{R}^P$
- While $\cancel{\|f(x_k)\| > \varepsilon}$ $\|d_k\| > \varepsilon$ and $k < k_{\max}$
  - Solve $(Jf(x_k)^T Jf(x_k))d_k = -Jf(x_k)^T f(x_k)$ ← LSQ system solution
  - Update $x_{k+1} = x_k + d_k$
  - Update $k \to k+1$

$Jf(x)\,d = -f(x)$

Convergence of the Gauss Newton method

We recall that $Jf(x)$ of rank P and $g(x)$ is strictly convex coercive

- Let $x_k \in \mathbb{R}^P$, then the direction $d_k = -(Jf(x_k)^T Jf(x_k))^{-1} Jf(x_k)^T f(x_k)$ satisfies

$$\langle \nabla g(x_k), d_k \rangle \leq 0.$$

descent direction

If $x_k \neq x^*$ then

$$\langle \nabla g(x_k), d_k \rangle < 0.$$

So d_k is a descent direction for g at x_k.

- If the sequence $(x_k)_k$ converges, then its limit is x^*.

Exercice

$$f(x) = 3x_1^2 + x_2^2 - 2x_1x_2 + x_1 + x_2 + 1$$

write in the quadratic form A, b, c

Exercice

$f : \mathbb{R}^2 \to \mathbb{R}$

$f(x_1, x_2) = 4(x_1^2 + x_2^2) - (x_1^2 + x_2^2)^2 \qquad X = (x_1, x_2)$

1) compute $\nabla f(X)$ and $Hf(X)$
2) compute the set of points $\{\nabla f(X) = 0\} = S$
3) Say if $X \in S$ is minimum or maximum or what?

$$\nabla f(X) = \begin{pmatrix} 8x_1 - 4x_1(x_1^2 + x_2^2) \\ 8x_2 - 4x_2(x_1^2 + x_2^2) \end{pmatrix} \quad Hf(x) = \begin{pmatrix} 8 - 12x_1^2 - 4x_2^2 & -8x_1x_2 \\ -8x_1x_2 & 8 - 12x_2^2 - 4x_1^2 \end{pmatrix}$$

$$\begin{pmatrix} 2x_1 = x_1(x_1^2 + x_2^2) \\ 2x_2 = x_2(x_1^2 + x_2^2) \end{pmatrix} \Leftrightarrow S = \{(0,0)\} \cup \left\{ \begin{array}{l} x_1^2 + x_2^2 = 2 \\ \text{circle of center } (0,0) \\ \text{radius } \sqrt{2} \end{array} \right\}$$

question 3 for tomorrow