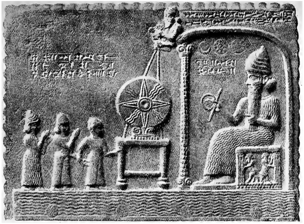
Metoda Newton

Scurt istoric: antichitate

Metoda babiloniana sau metoda lui Heron: dandu-se un numar $c \in \mathbb{R}$, aceasta metoda consta in calcularea iterativa a lui $x = \sqrt{c} \Leftrightarrow x^2 - c = 0$:

$$\begin{aligned} x_{k+1} &= \frac{1}{2}\left(x_k + \frac{c}{x_k}\right) \\ &= x_k - \frac{1}{2x_k}(x_k^2 - c) \end{aligned}$$

Este considerata drept precursor (caz special) al metodei Newton. Utilizata de babilonieni, descrisa prima data de catre Heron din Alexandria.

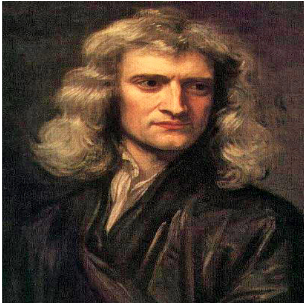


Scurt istoric: secolul al XVII-lea

In 1669, Isaac Newton imbunatat-este o tehnica a perturbatiilor dez-voltata de Francois Viete pentru a afla solutiile unei ecuatii $F(x) = 0$, unde $F(x)$ este un polinom. Avand un punct de pornire x_0, ideea principala este linearizarea:

$$F(x_0 + h) = F(x_0) + F'(x_0)h$$

Astfel, sa se gaseasca h astfel incat $F(x_0 + h) = 0$, ce conduce la iteratia :



$$x_{k+1} = x_k - F'(x_k)^{-1}F(x_k) \quad (1)$$

Metoda originala a lui Newton a fost pur algebrica. In 1669, Joseph Raphson considera ca $F(x)$ nu trebuie sa fie neaparat polinom si prezinta forma generala (1) utilizand conceptul de derivata. De aceea, metoda se numeste metoda Newton-Raphson.

Metoda Newton in Optimizare

Consideram $f : \mathbb{R}^n \to \mathbb{R}$ si problema de optimizare aferenta:

$$\min_{x \in \mathbb{R}^n} f(x)$$

Din conditiile de optimalitate de ordinul I pentru probleme neconstranse amintim: x^* este punct de minim local daca $\nabla f(x^*) = 0$ si $\nabla^2 f(x^*) \succ 0$, unde $\nabla^2 f(x^*)$ denota Hessiana lui $f(x)$ in punctul x^*.

Astfel, pentru a afla x^* trebuie sa mai intai aflam solutia ecuatiei:

$$F(x) = \nabla f(x) = 0$$

• **Interpretare**: Aplicand metoda lui Newton-Raphson in acest caz, rezulta iteratia:

$$x_{k+1} = x_k - \left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$$

Metoda Newton in Optimizare

Fiind metoda iterativa, metoda lui Newton se poate scrie drept:

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

unde $d_k = -\left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$ se numeste directia Newton

• **Interpretare**: daca $\nabla f(x)^2 \succ 0$, atunci $\langle d_k, \nabla f(x_k) \rangle < 0$, i.e d_k este o directie de descrestere.

• **Interpretare**: metoda Newton poate fi obtinuta din aproximarea Taylor de ordinul doi a functiei obiectiv f:

$$f(x_{k+1}) \approx f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{1}{2}(x_{k+1} - x_k)^T \nabla^2 f(x_k)(x_{k+1} - x_k)$$

Urmatoarea iteratie, x_{k+1}, trebuie sa minimizeze aproximarea Taylor, de unde rezulta:

$$x_{k+1} = \arg\min_y \underbrace{f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2}(y - x_k)^T \nabla^2 f(x_k)(y - x_k)}_{q(y)}$$

Metoda Newton in Optimizare

Daca $\nabla^2 f(x_k) \succ 0$, atunci $q(y)$ este o functie patratica strict convexa. Din conditiile de optimalitate pentru probleme QP strict convexe, rezulta:

$$\nabla q(y) = 0 \Rightarrow \nabla f(x_k) + \nabla^2 f(x_k)(y - x_k) = 0$$

Din moment ce $y = x_{k+1}$, prin rezolvarea ecuatiei anterioare in y rezulta din nou iteratia:

$$x_{k+1} = x_k - (\nabla^2 f(x_k))^{-1} \nabla f(x_k)$$

Observatie, din moment ce directia Newton $d_k = x_{k+1} - x_k$, atunci se poate exprima drept:

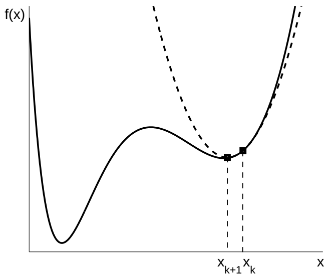
$$d_k = \arg\min_d f(x_k) + \nabla f(x_k)^T d + \frac{1}{2} d^T \nabla^2 f(x_k) d.$$

Din nou, utilizand conditiile de optimalitate, rezulta:

$$d_k = -\left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$$

Metoda Newton in Optimizare

Iteratie metoda Newton prin aproximarea patratica Taylor:



Observatie: metoda Newton pentru functii $f : \mathbb{R} \to \mathbb{R}$ este chiar metoda Newton de interpolare din cursul III:

$$
\begin{aligned}
x_{k+1} &= \arg\min_x q(x) = \arg\min_x f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2} f''(x_k)(x - x_k)^2 \\
&= x_k - \left(f''(x_k)\right)^{-1} f'(x_k)
\end{aligned}
$$

Convergenta locala a Metodei Newton

Teorema (rata de convergenta locala a metodei Newton):

- fie $f \in C^2$ si x^* un minim local ce satisface $\nabla f(x^*) = 0$ si $\nabla^2 f(x^*) \succ 0$
- fie o constanta $m > 0$ astfel incat: $\nabla^2 f(x^*) \succeq mI_n$
- presupunem ca $\nabla^2 f(x)$ este Lipschitz cu constanta $M > 0$, i.e.

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq M\|x - y\| \;\; \forall x, y \in \mathrm{dom} f$$

- presupunem ca punctul initial x_0 este suficient de aproape de x^*, i.e. $\|x_0 - x^*\| \leq \frac{2}{3} \cdot \frac{m}{M}$

Atunci iteratia Newton $x_{k+1} = x_k - (\nabla^2 f(x_k))^{-1} \nabla f(x_k)$ converge la x^* cu rata patratica, i.e.

$$\|x_{k+1} - x^*\| \leq \frac{3M}{2m} \|x_k - x^*\|^2 \quad \forall k \geq 0$$

Prima demonstratie data de Kantorovich in 1948!

Convergenta locala a Metodei Newton

Demonstratie: x^* este un minim local $\rightarrow \nabla f(x^*) = 0$.
Din teorema lui Taylor in forma integrala avem:

$$\nabla f(x_k) = \nabla f(x^*) + \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau.$$

Se obtine:

$$x_{k+1} - x^* = x_k - x^* - (\nabla^2 f(x_k))^{-1} \nabla f(x_k)$$
$$= (\nabla^2 f(x_k))^{-1} [\nabla^2 f(x_k)(x_k - x^*) - \nabla f(x_k) + \nabla f(x^*)]$$
$$= (\nabla^2 f(x_k))^{-1} [\nabla^2 f(x_k)(x_k - x^*) - \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau]$$
$$= (\nabla^2 f(x_k))^{-1} \int_0^1 [\nabla^2 f(x_k)(x_k - x^*) - \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau]$$
$$= (\nabla^2 f(x_k))^{-1} \int_0^1 [\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*))](x_k - x^*) d\tau.$$

Convergenta locala a Metodei Newton

Deoarece $\|\nabla^2 f(x_k) - \nabla^2 f(x^*)\| \leq M\|x_k - x^*\|$, avem:

$$-M\|x_k - x^*\| I_n \preceq \nabla^2 f(x_k) - \nabla^2 f(x^*) \preceq M\|x_k - x^*\| I_n.$$

Mai mult, vom avea:

$$\nabla^2 f(x_k) \succeq \nabla^2 f(x^*) - M\|x_k - x^*\| I_n \succeq mI_n - M\|x_k - x^*\| I_n \succ 0,$$

sub ipoteza ca $\|x_k - x^*\| \leq \frac{2}{3}\frac{m}{M}$, de unde rezulta:

$$0 \prec (\nabla^2 f(x_k))^{-1} \preceq \frac{1}{m - M\|x_k - x^*\|} I_n.$$

Concluzionam urmatoarele:

$$\|x_{k+1} - x^*\| = \|(\nabla^2 f(x_k))^{-1}\| \cdot \|\int_0^1 \nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau\| \cdot$$

$$\leq \frac{1}{m - M\|x_k - x^*\|} \int_0^1 M(1-\tau)\|x_k - x^*\| d\tau \|x_k - x^*\|$$

$$\leq \frac{1}{m - M\|x_k - x^*\|} \int_0^1 M(1-\tau) d\tau \|x_k - x^*\|^2$$

Convergenta locala a Metodei Newton

Prin inductie se arata usor ca daca $\|x_0 - x^*\| \leq 2m/3M$, atunci $\|x_k - x^*\| \leq 2m/3M$ pentru orice $k \geq 0$.
Observam ca $\frac{1}{m - M\|x_k - x^*\|} \frac{M}{2} \leq \frac{3M}{2m} < \infty$ si deci obtinem $\|x_{k+1} - x^*\| \leq \frac{3M}{2m} \|x_k - x^*\|^2$.

Observatii: Consideram $f(x)$ patratica, strict convexa, i.e. $f(x) = \frac{1}{2} x^T Q x + q^T x$, unde $Q \succ 0$. Din conditiile de optimalitate:

$$\nabla f(x^*) = Qx^* + q = 0 \Rightarrow x^* = -Q^{-1} q$$

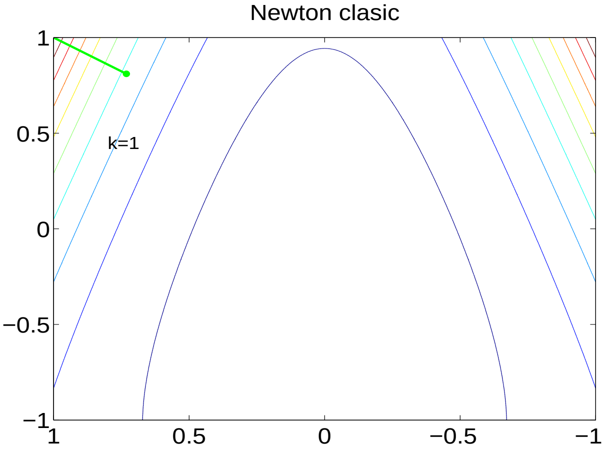
Pornind dintr-un punct x_0, si aplicand metoda Newton, rezulta:

$$x_1 = x_0 - \left(\nabla^2 f(x_0)\right)^{-1} \nabla f(x^0) = x_0 - Q^{-1}(Qx_0 + q) = -Q^{-1} q = x^*,$$

deci pentru probleme patratice strict convexe metoda converge intr-un singur pas.
Dar metoda Newton necesita calculul inversei $\nabla^2 f(x)^{-1}$, **operatie costisitoare** $\mathcal{O}(n^3)$ pentru probleme de dimensiuni mari.

Convergenta locala a Metodei Newton

Exemplu metoda Newton cu pas variabil ales in trei variante, aplicata pe $f\colon \mathbb{R}^2 \to \mathbb{R}$, $f(x) = e^{x_1+3x_2-0.1} + e^{x_1-3x_2-0.1} + e^{-x_1-0.1}$.



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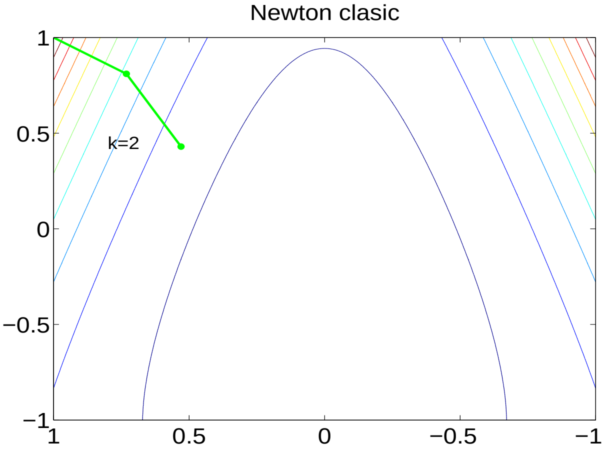

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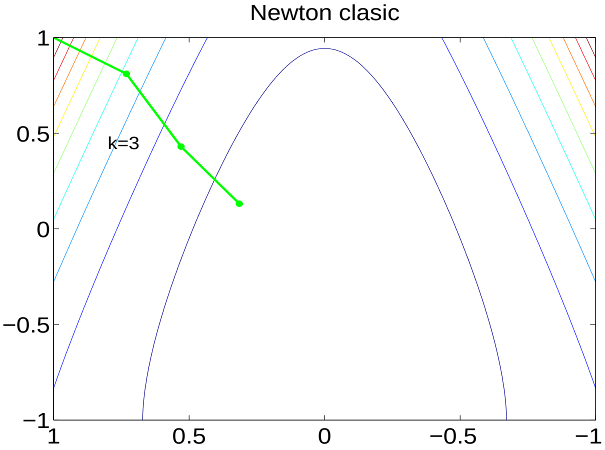

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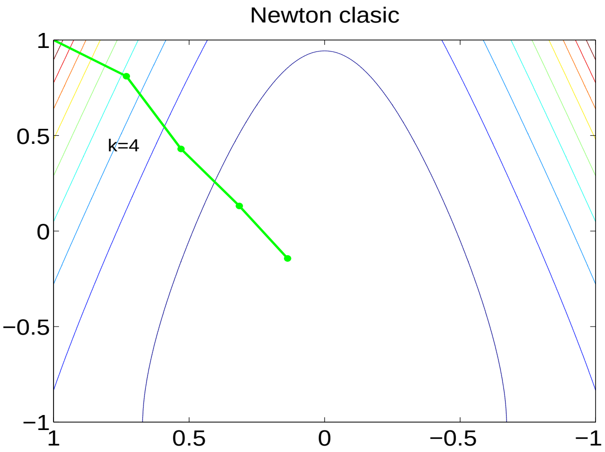

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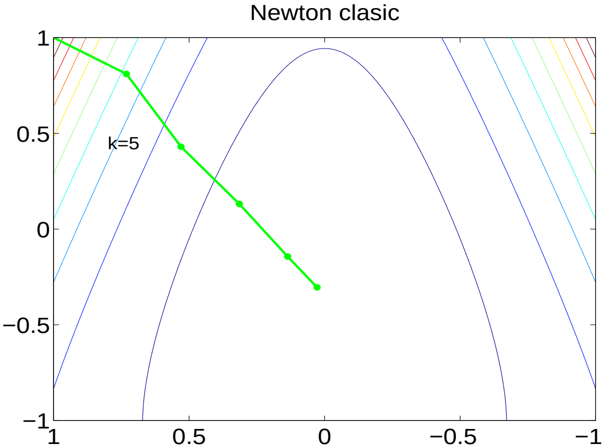

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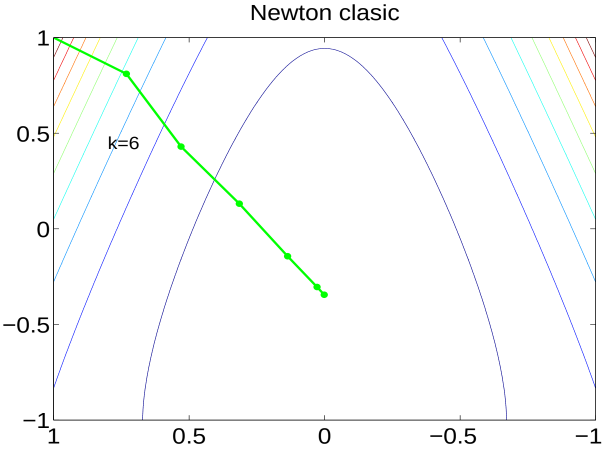

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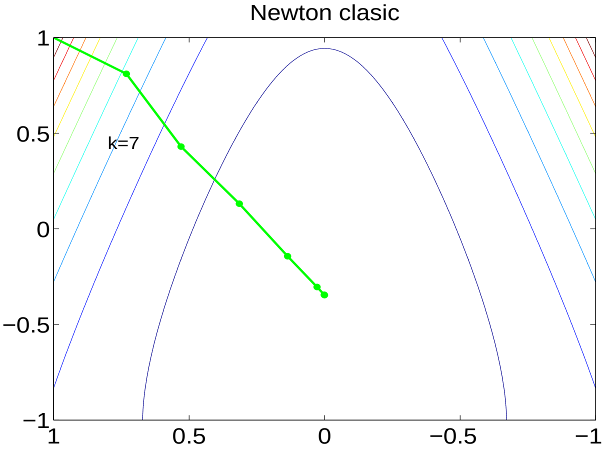

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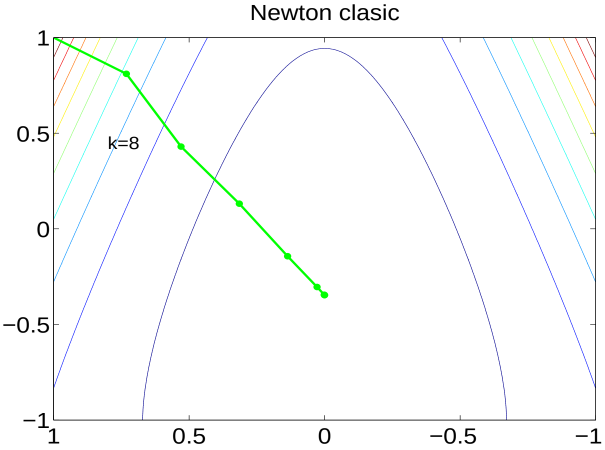

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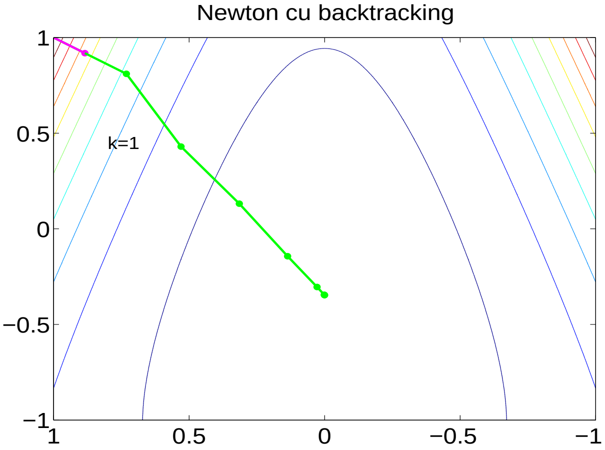

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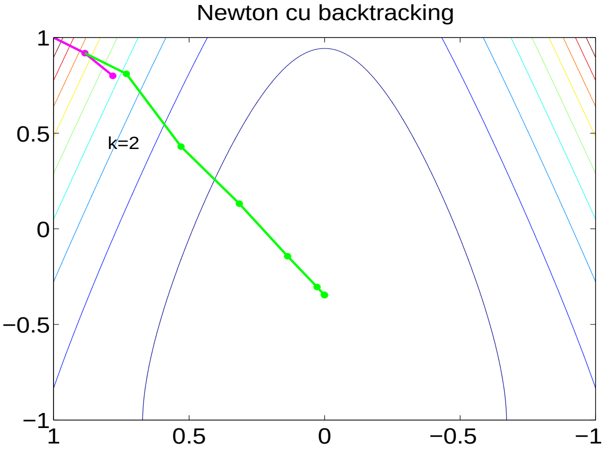

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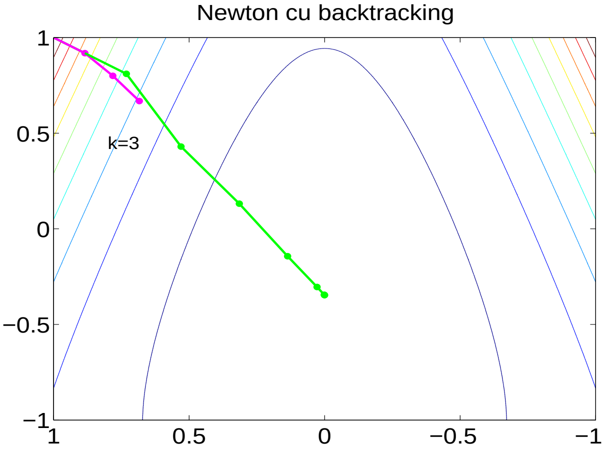

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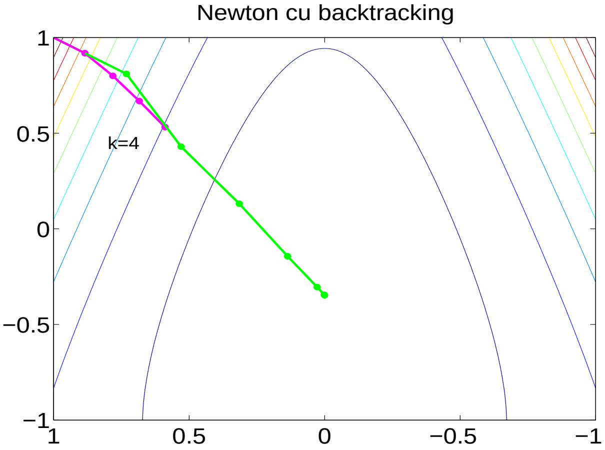

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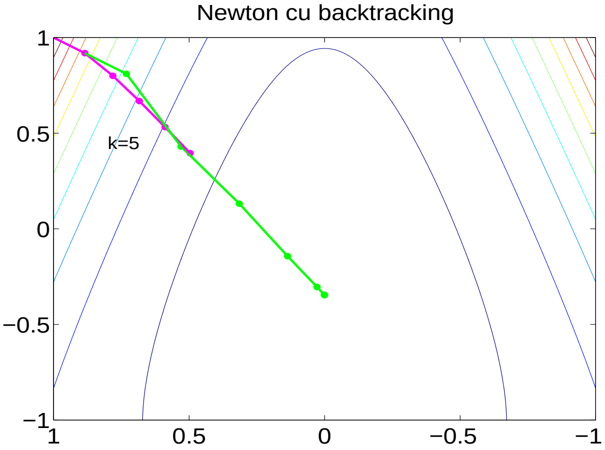

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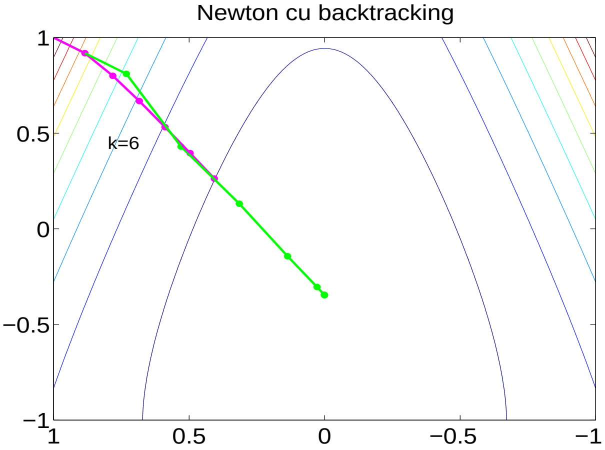

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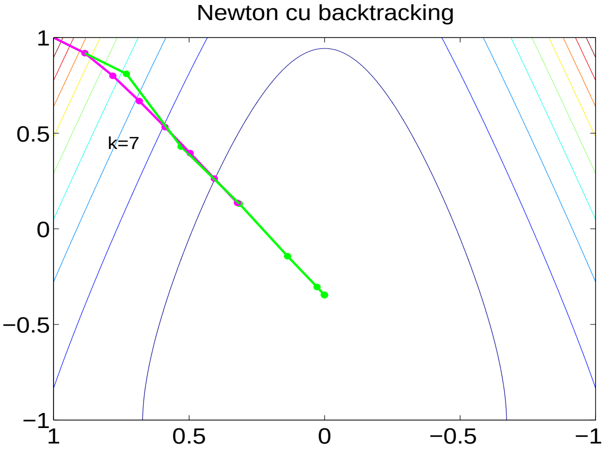

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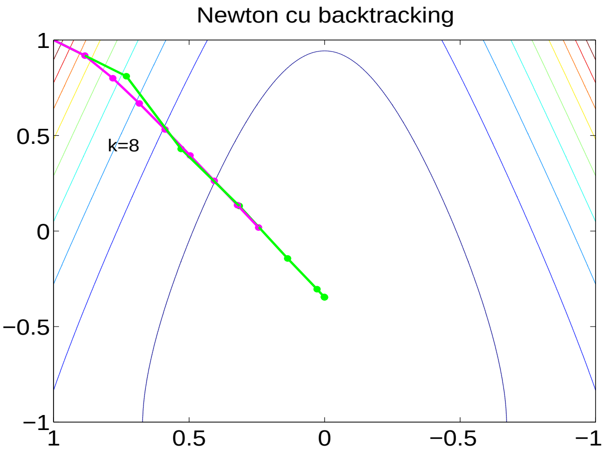

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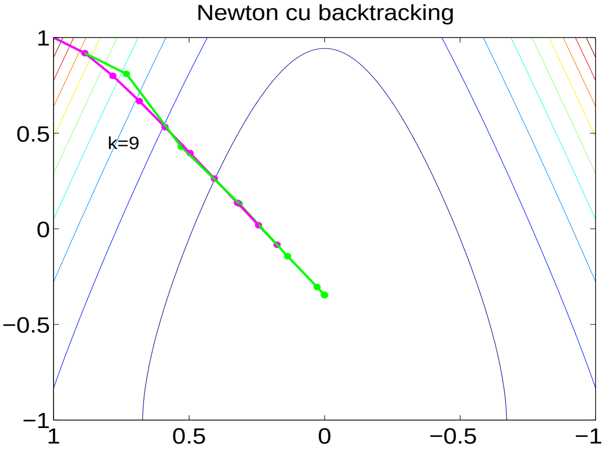

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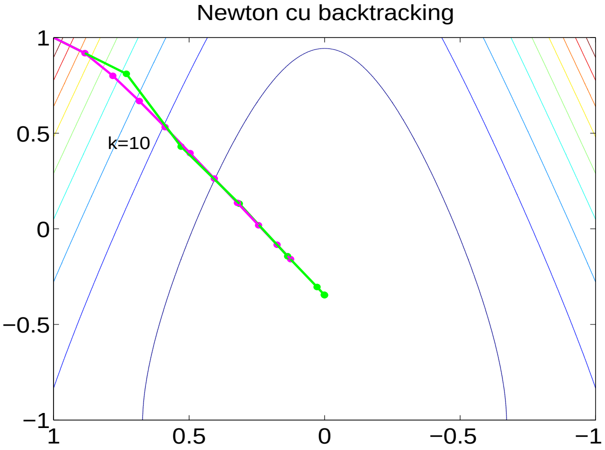

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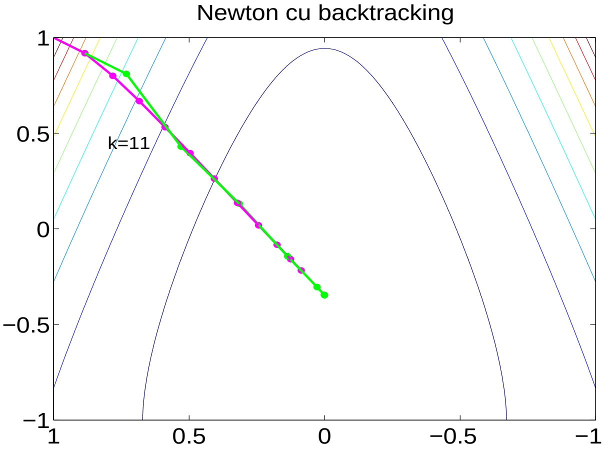

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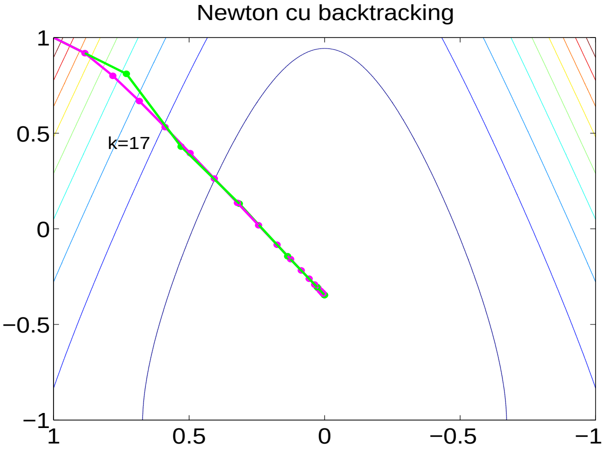

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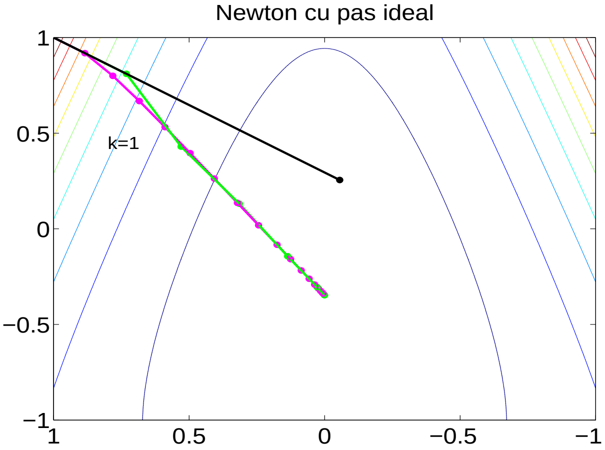

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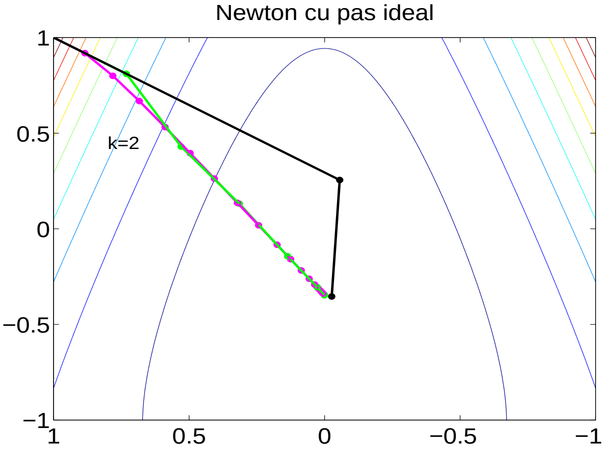

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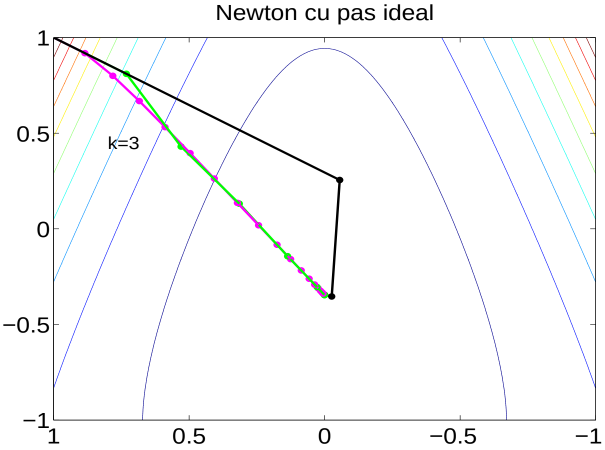

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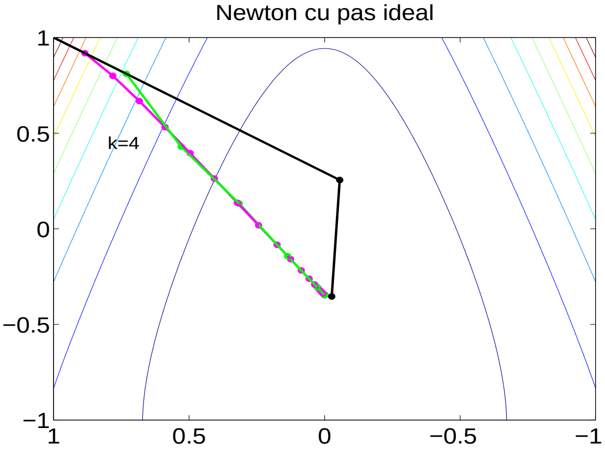

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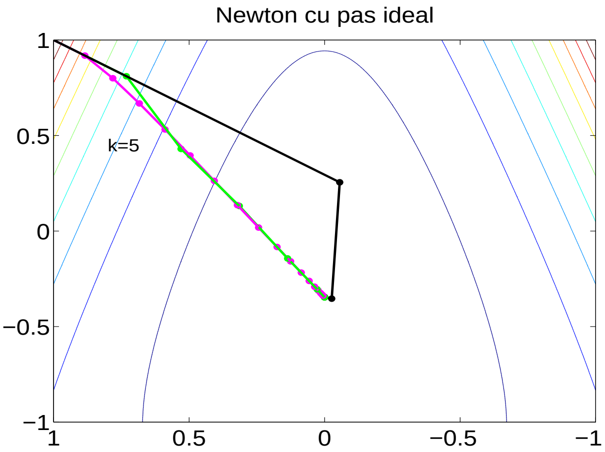

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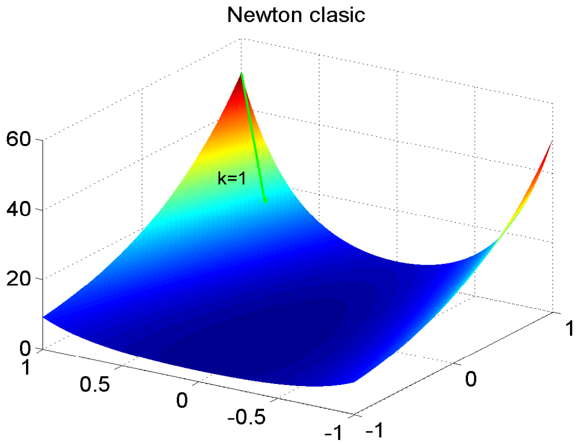

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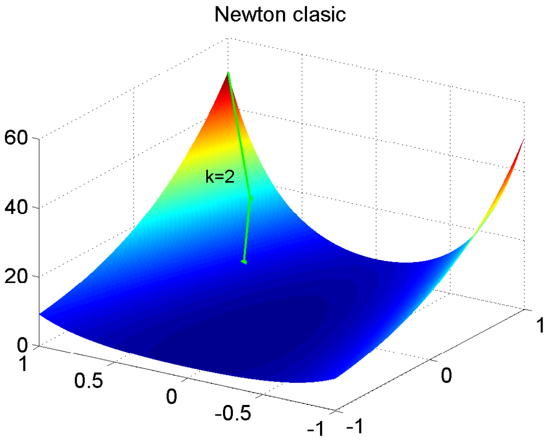

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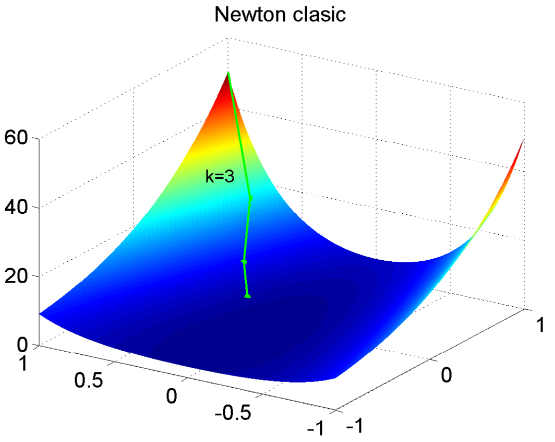

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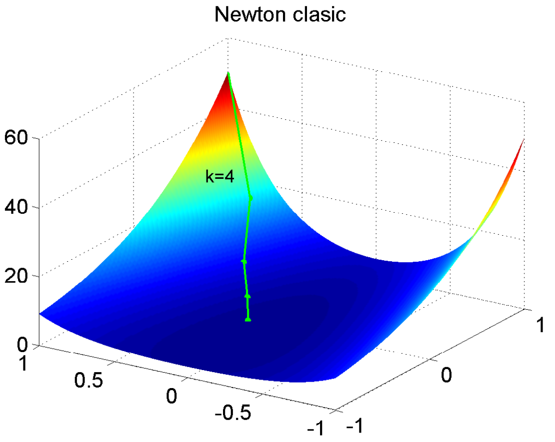

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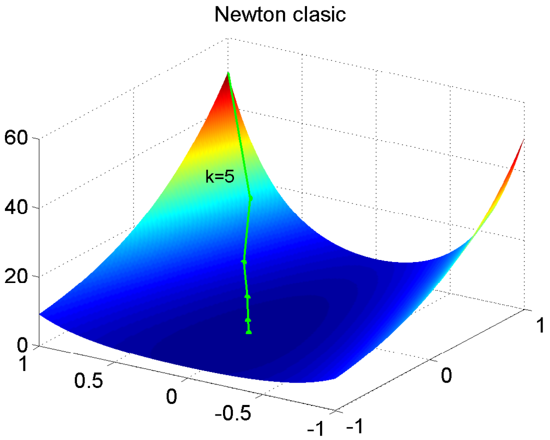

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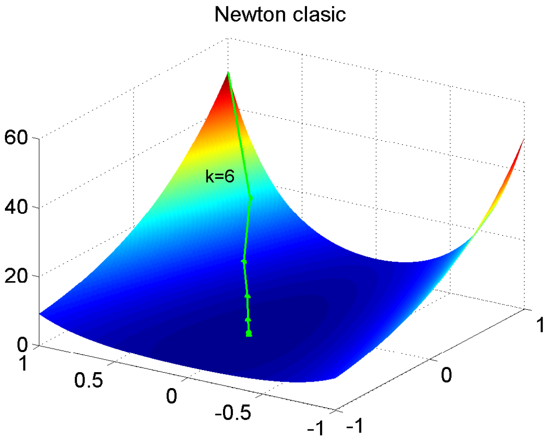

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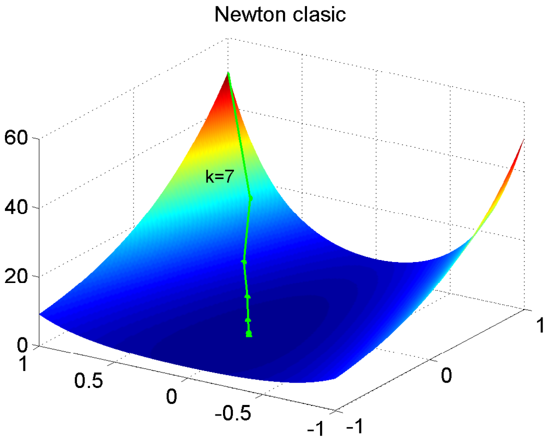

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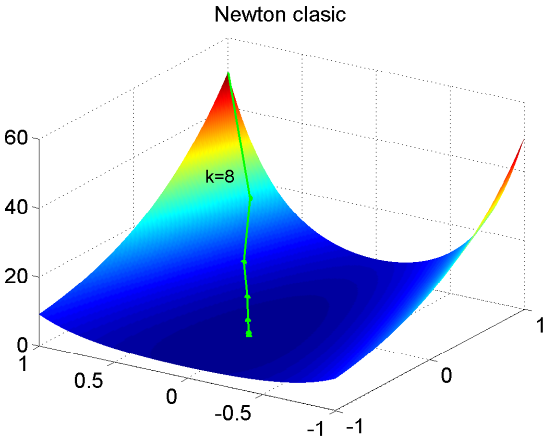

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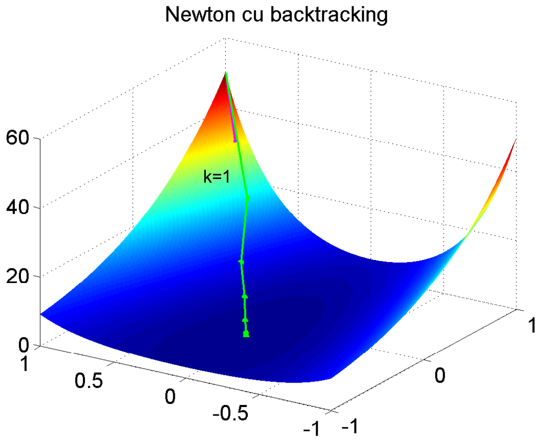

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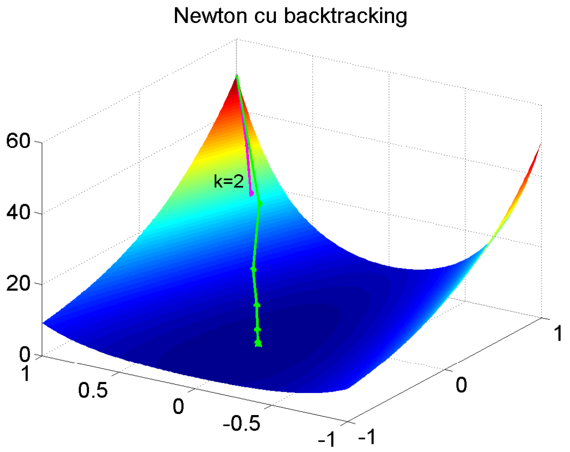

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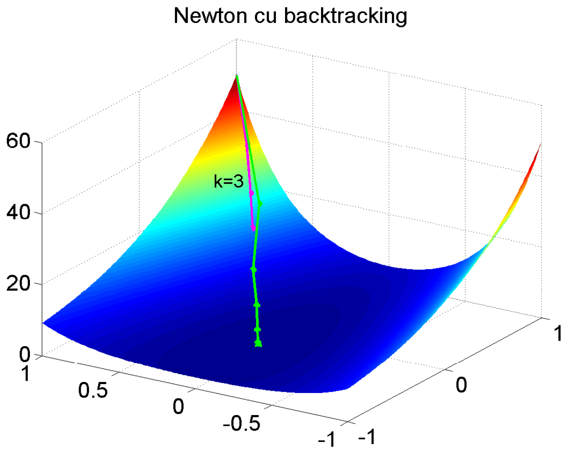

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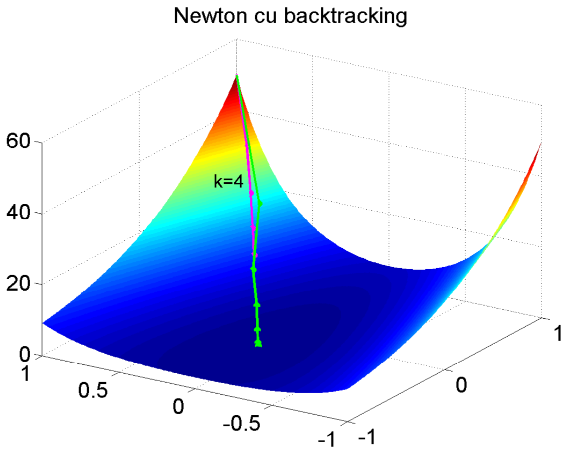

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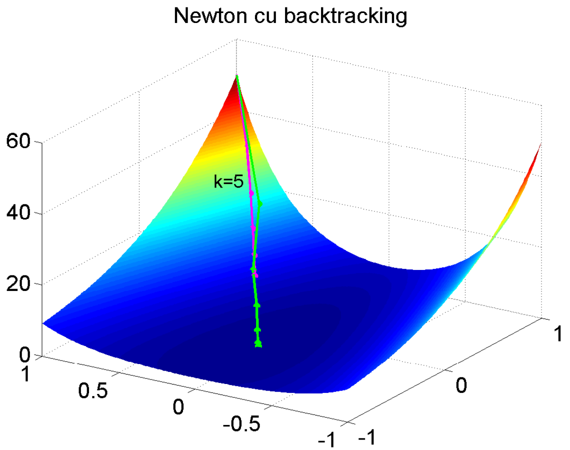

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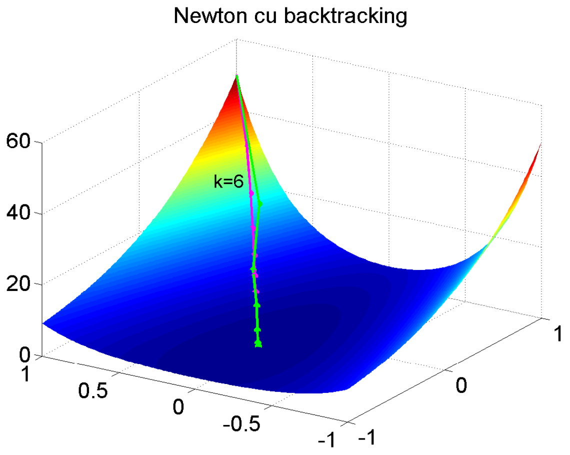

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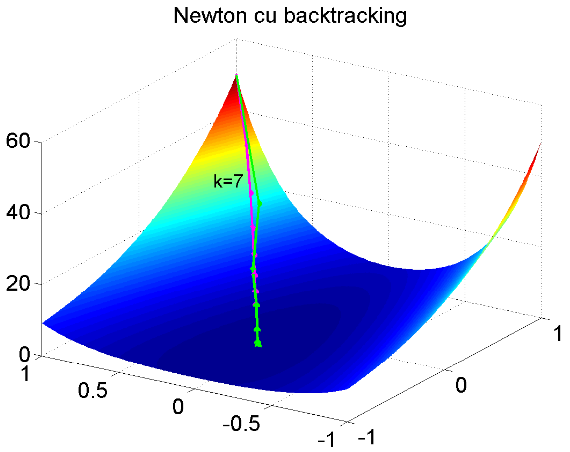

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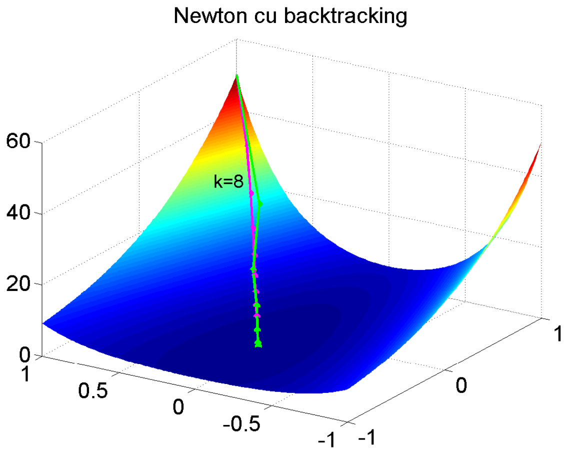

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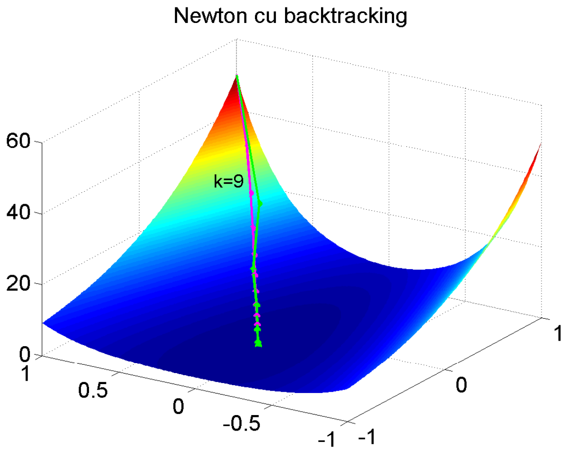

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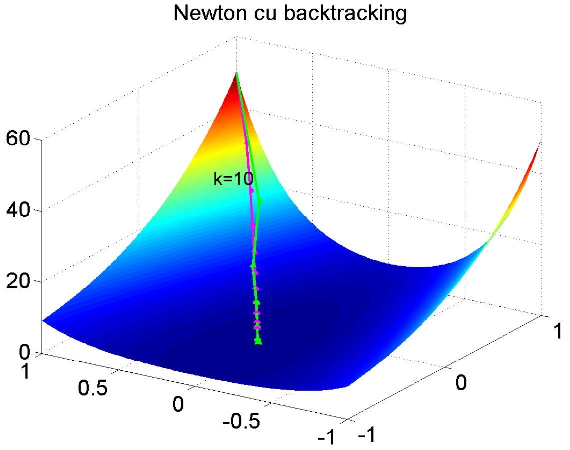

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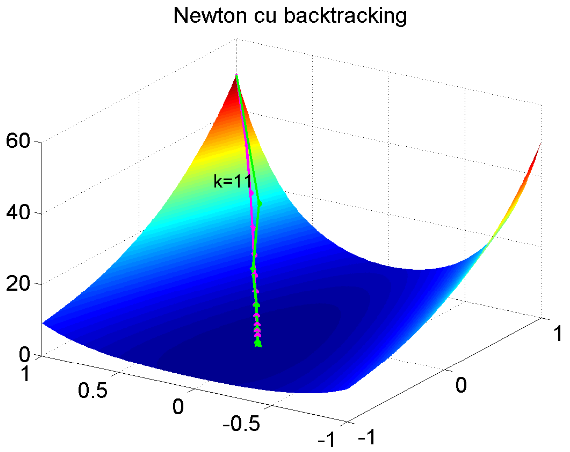

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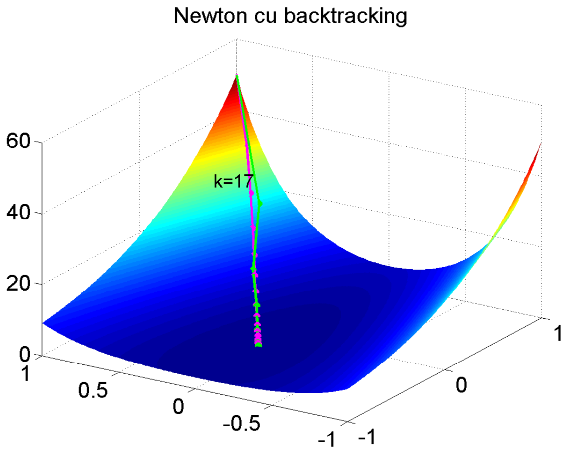

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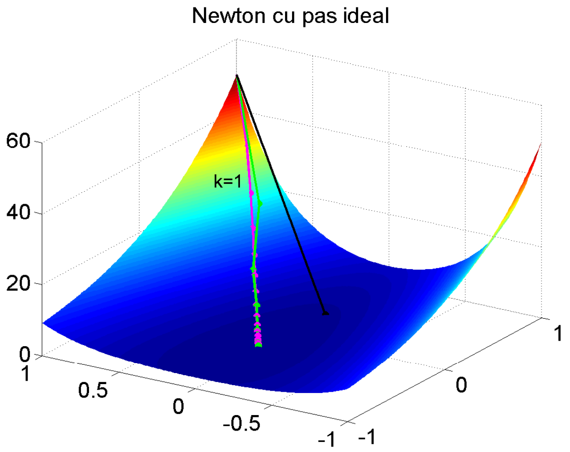

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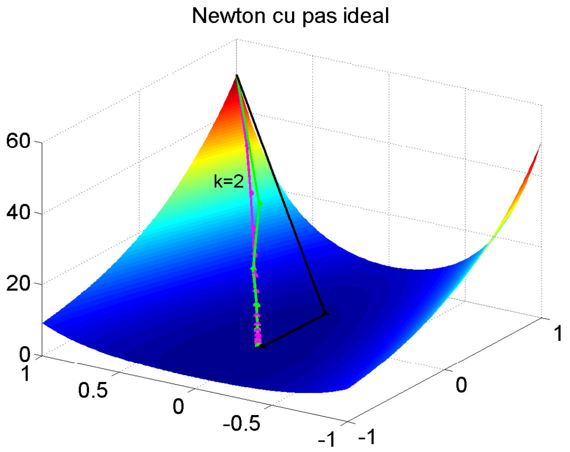

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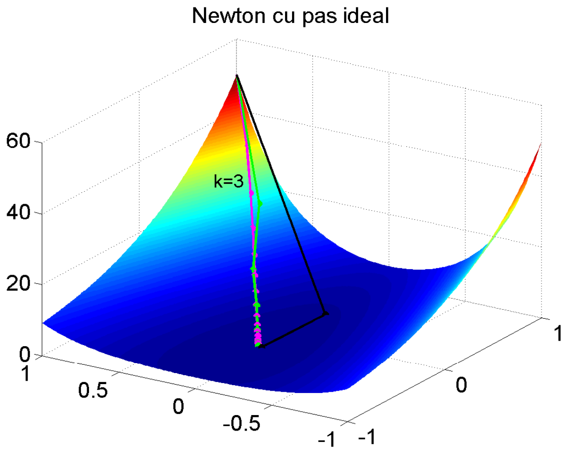

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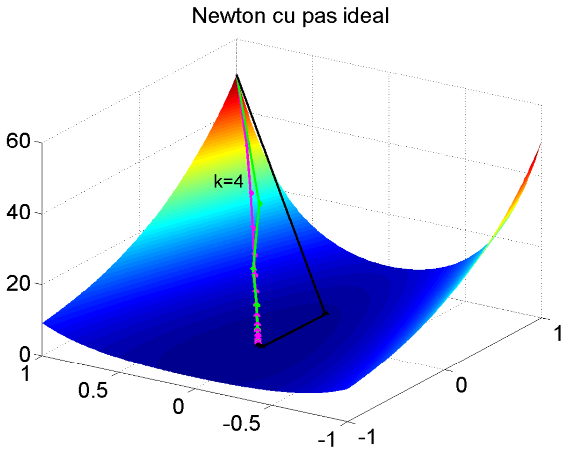

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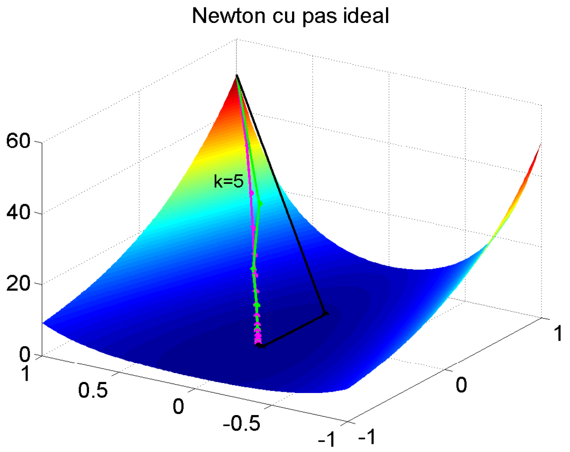

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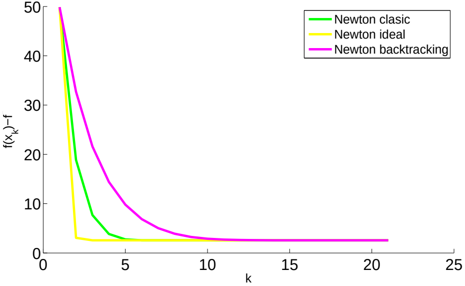
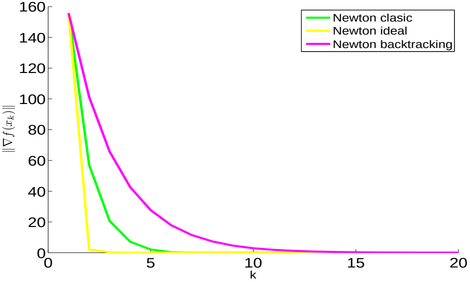




Convergenta globala a Metodei Newton

Daca pornim dintr-un punct x_0 ce nu se afla in vecinatatea lui x^*, metoda Newton trebuie modificata pentru a asigura convergenta:

$$x_{k+1} = x_k - \alpha_k \left(\nabla^2 f(x_k)\right)^{-1} \nabla f(x_k)$$

Pasul α_k se poate alege ideal (i.e. $\alpha_k = \min_{\alpha \geq 0} f(x_k + \alpha_k d_k)$) sau prin metoda backtracking

Teorema (convergenta globala a metodei Newton):

- Fie functia obiectiv $f \in \mathcal{C}^2$ marginita inferior si cu gradientul ∇f Lipschitz
- Consideram metoda Newton cu pas variabil α_k ales prin backtracking: $x_{k+1} = x_k - \alpha_k(\nabla^2 f(x_k))^{-1}\nabla f(x_k)$
- Presupunem ca Hessiana satisface conditia $\beta_1 I_n \preceq (\nabla^2 f(x))^{-1} \preceq \beta_2 I_n$, unde $0 < \beta_1 \leq \beta_2$.

Atunci, metoda Newton produce un sir x_k cu proprietatea ca $\nabla f(x_k) \to 0$.

Metoda Newton versus metoda gradient

- Metoda gradient cu pas α_k se obtine prin aproximarea Taylor, unde insa $\nabla^2 f(x_k)$ este inlocuita cu $\frac{1}{\alpha_k} I_n$:

$$
\begin{aligned}
x_{k+1} &= x_k - \alpha_k \nabla f(x_k) \\
&= \arg\min_y f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2\alpha_k}(y - x_k)^T I_n (y - x_k)
\end{aligned}
$$

$\Longrightarrow$ complexitate pe iteratie $\mathcal{O}(n)$ plus costul evaluarii $\nabla f(x)$!

- Metoda Newton cu pas α_k se obtine prin aproximarea Taylor de ordin II:

$$
\begin{aligned}
x_{k+1} &= x_k - \alpha_k (\nabla^2 f(x_k))^{-1} \nabla f(x_k) \\
&= \arg\min_y f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2\alpha_k}(y - x_k)^T \nabla^2 f(x_k)(y - x_k)
\end{aligned}
$$

$\Longrightarrow$ complexitate pe iteratie $\mathcal{O}(n^3)$ plus costul evaluarii $\nabla f(x)$ si $\nabla^2 f(x)$!

Metoda Newton versus metoda gradient

$$\min_{x \in \mathbb{R}^2} f(x) \quad (= 10x_1^6 + 30x_2^6 + x_1^2 + 50x_2^2)$$

```
function [] = gradient-Newton-ideal(x0,eps)
obj = @(x)10x_1^6 + 30x_2^6 + x_1^2 + 50x_2^2;
gradient = @(x)[60x_1^5 + 2x_1 ; 180x_2^5 + 100x_2];
hessiana = @(x)[300x_1^4 + 2   0; 0   900x_2^4 + 100];
%% Metoda Gradient cu pas ideal
x = x0;
trajectory_g = [x0];
while (norm(gradient(x)) > eps)
    grad = gradient(x);
    obj_α = @(α) obj(x - α grad);
    α* = fminbnd(obj_α, 0, 1);

    x = x - α* gradient(x);
    trajectory_g = [trajectory_g x];
end
```

Metoda Newton versus metoda gradient

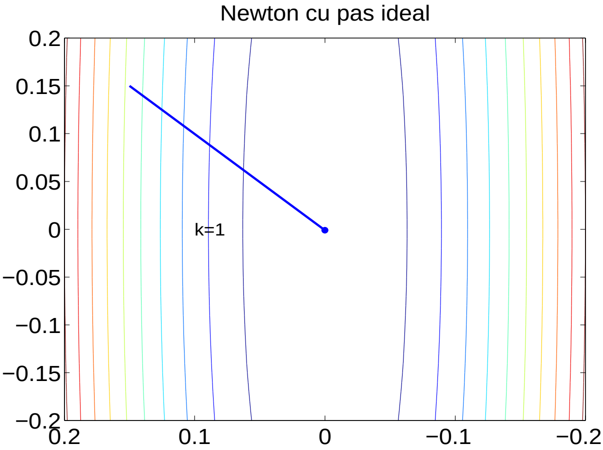
```
%% Metoda Newton cu pas ideal
x=x0;
trajectory_n = [x0];
while (norm(gradient(x)) > eps)
    grad = gradient(x);
    hess = hessiana(x);
    d-newton = inv(hess)* grad;
    obj_α = @(α) obj(x - α *d-newton);
    α* = fminbnd(obj_α, 0, 1);
    x = x - α* d-newton;
    trajectory_n = [ trajectory_n x];
end
```

Metoda Newton versus metoda gradient

```
x = −0.2 : 0.1 : 0.2;
y = −0.2 : 0.1 : 0.2;
[X,Y] = meshgrid(x,y);
Z = 10*X.^6 + 30*Y.^6 + X.^2 + 50*Y.^2;
figure
plot(trajectory_g(1,:),trajectory_g(2,:),'r+-','LineWidth',3);
hold on
plot(trajectory_n(1,:),trajectory_n(2,:),'k*--','LineWidth',3);
legend('Gradient Method','Newton Method');
hold on
contour(X,Y,Z,'ShowText','on','LineWidth',2);
end
```

Metoda Newton versus metoda gradient

Comparatie intre metoda Newton si metoda gradient, ambele cu pas ideal, pentru $f : \mathbb{R}^2 \to \mathbb{R}$, $f(x) = 10x_1^6 + 30x_2^6 + x_1^2 + 50x_2^2$



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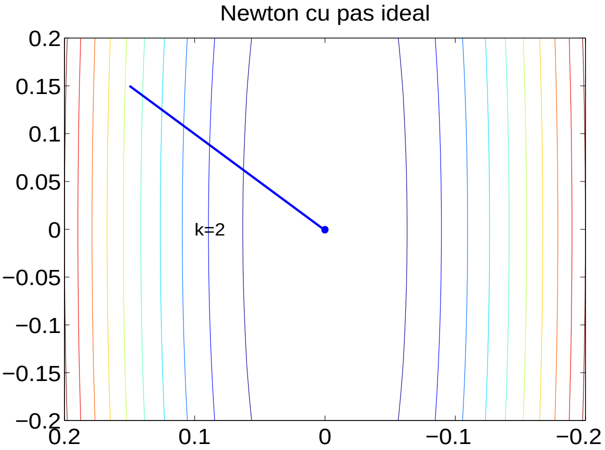

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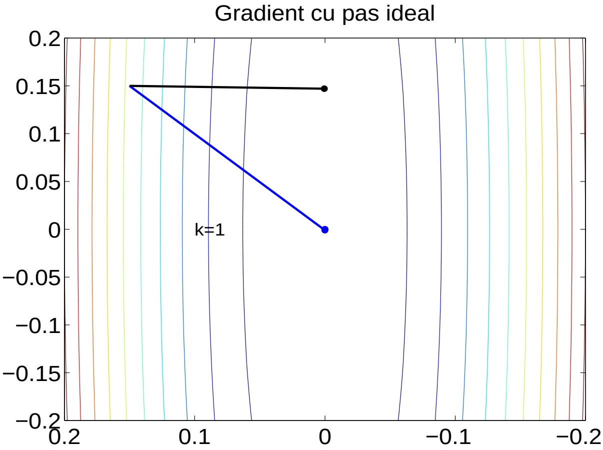

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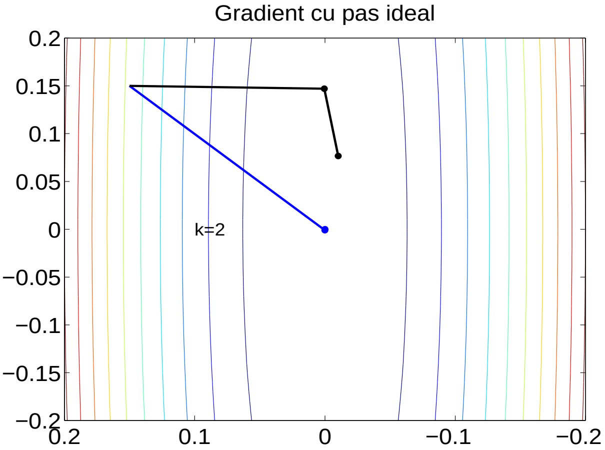

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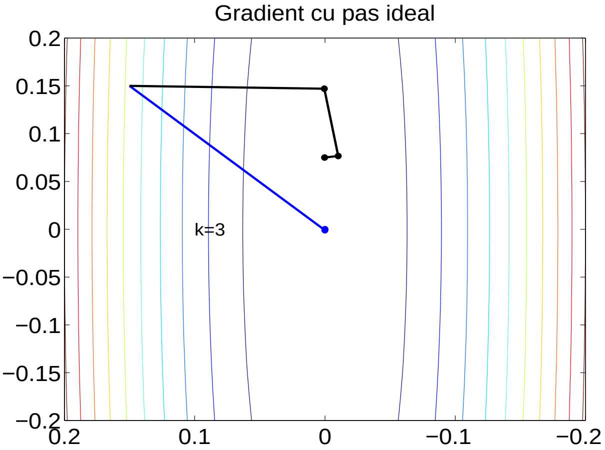

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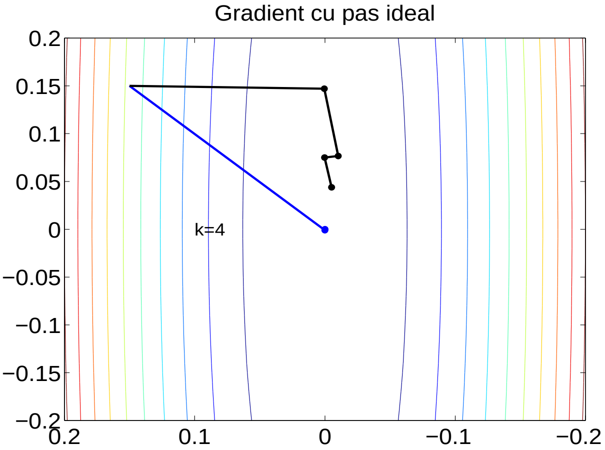

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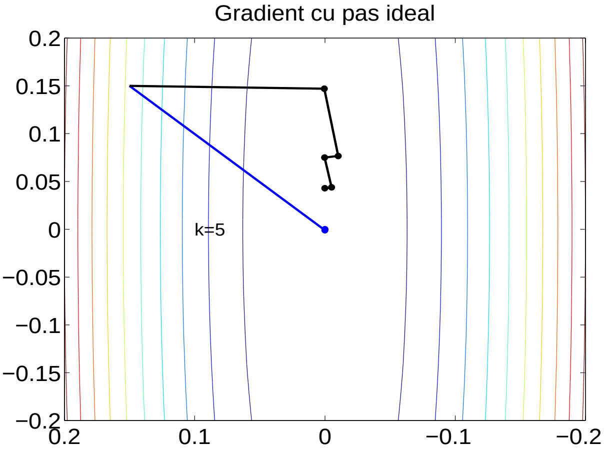

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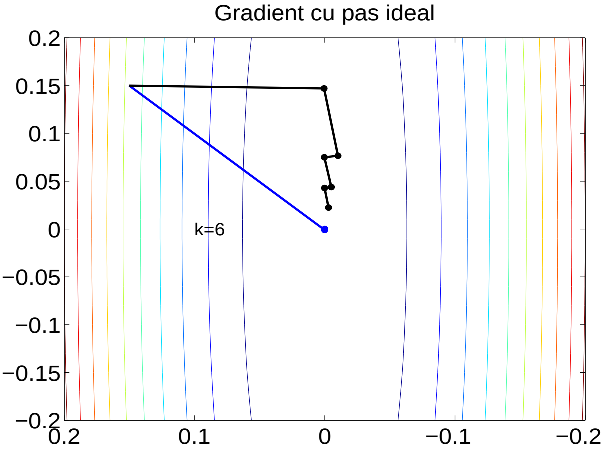

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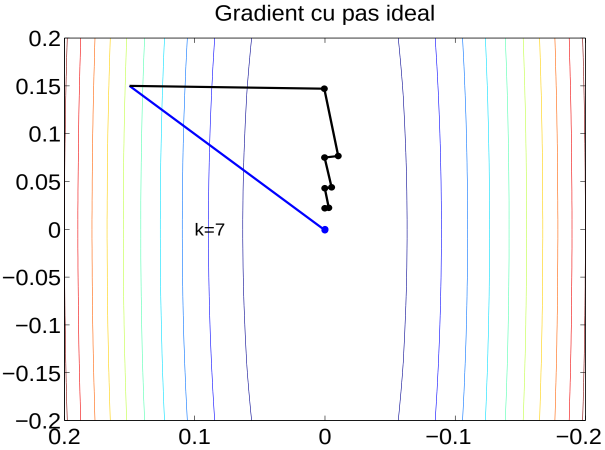

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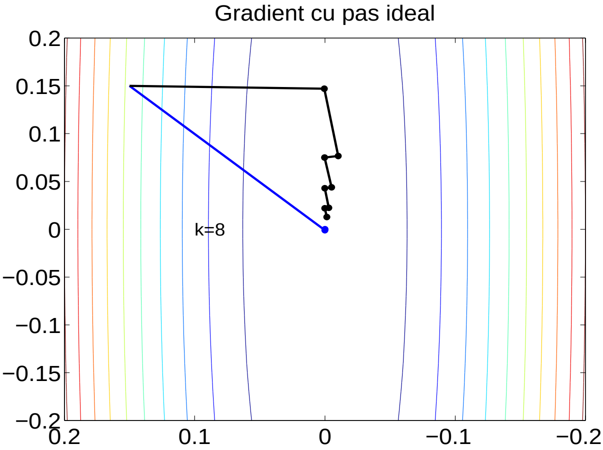

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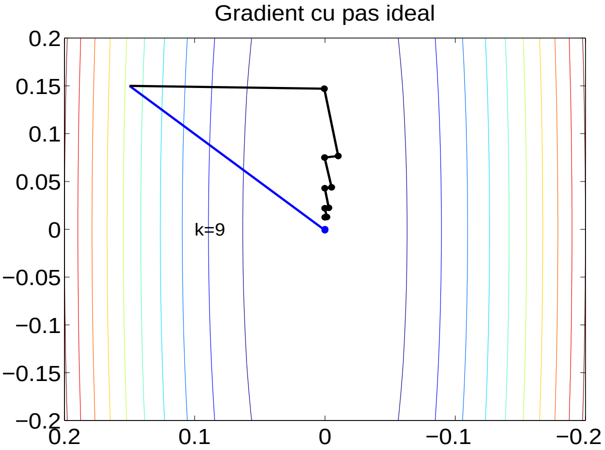

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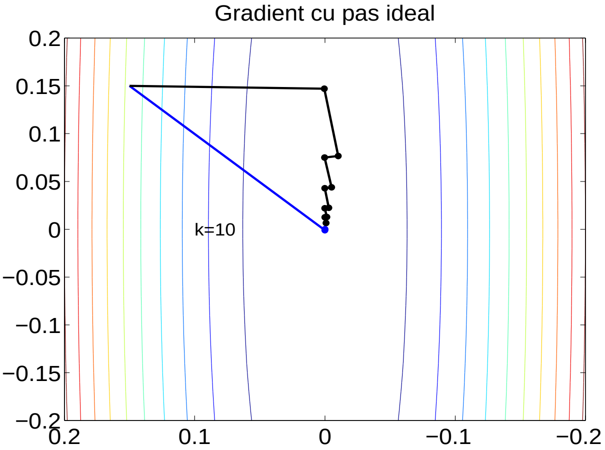

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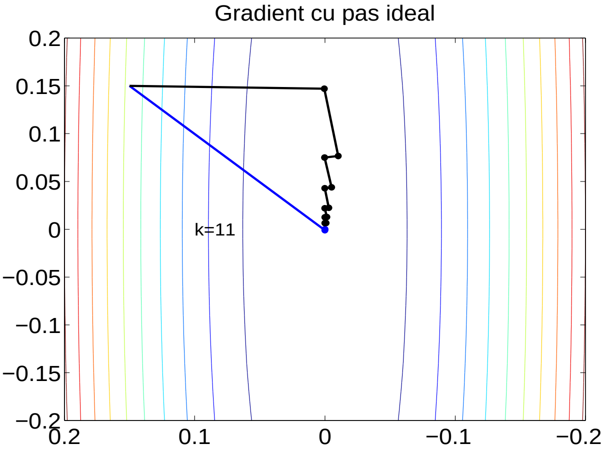

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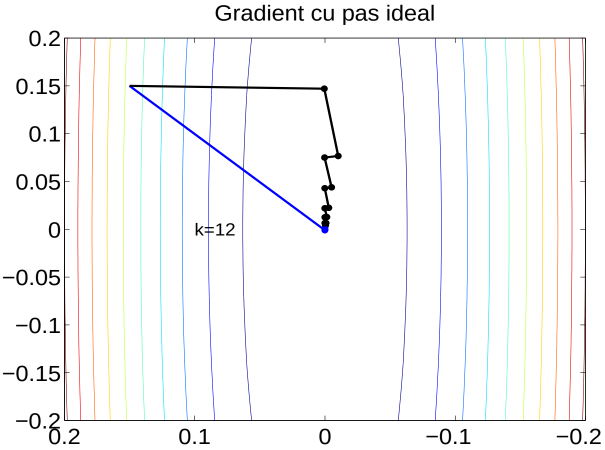

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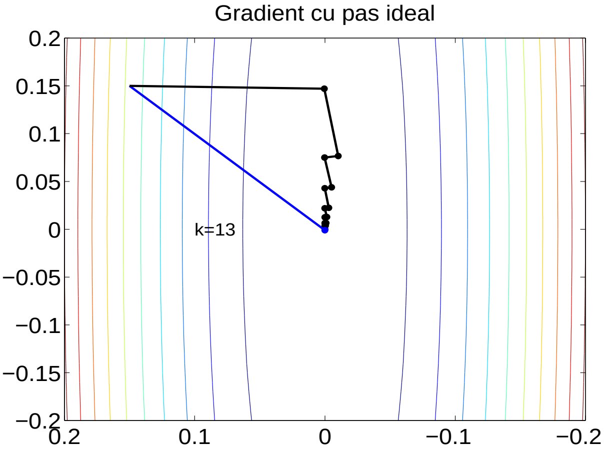

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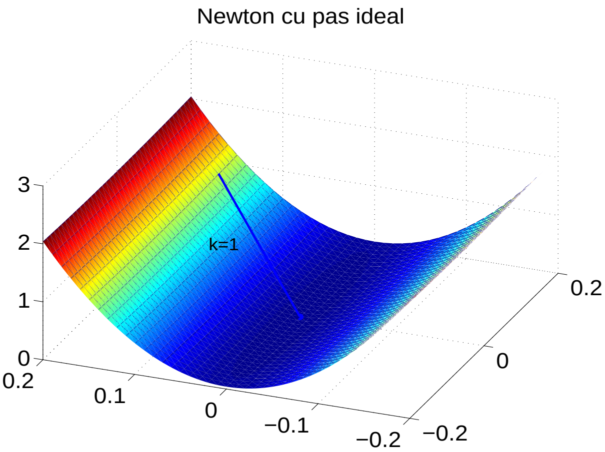

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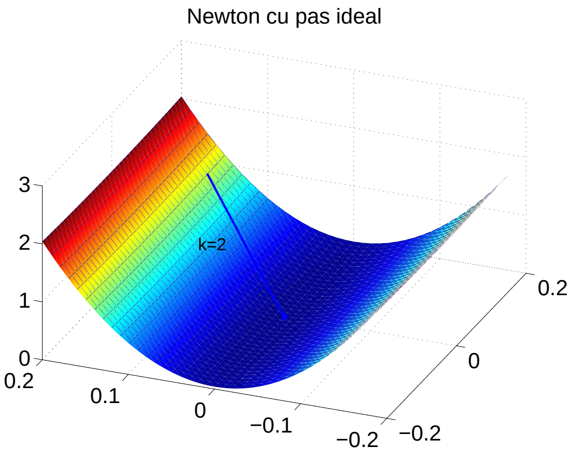
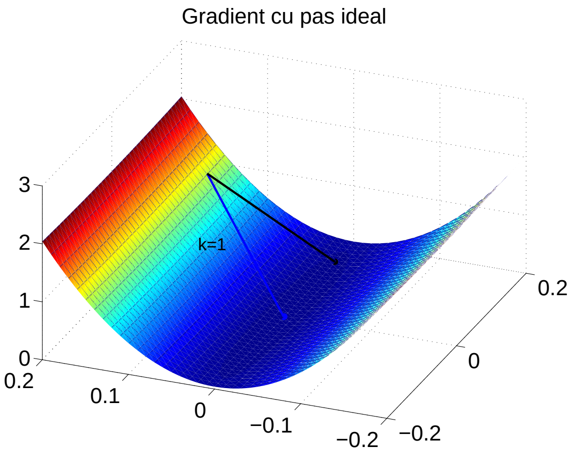
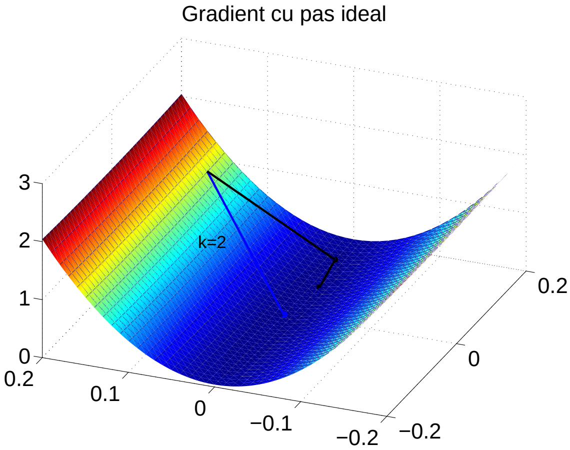


Metoda Newton versus metoda gradient



Metoda Newton versus metoda gradient



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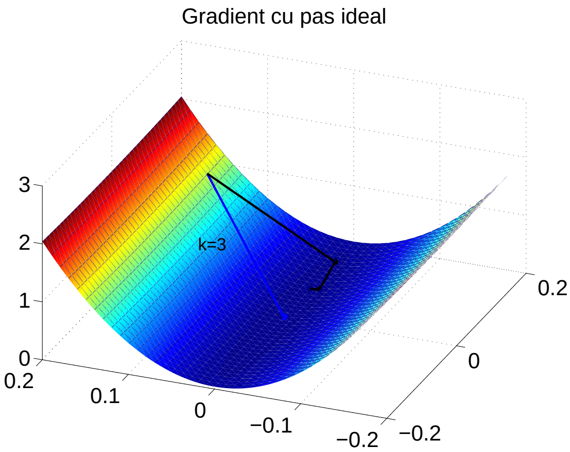
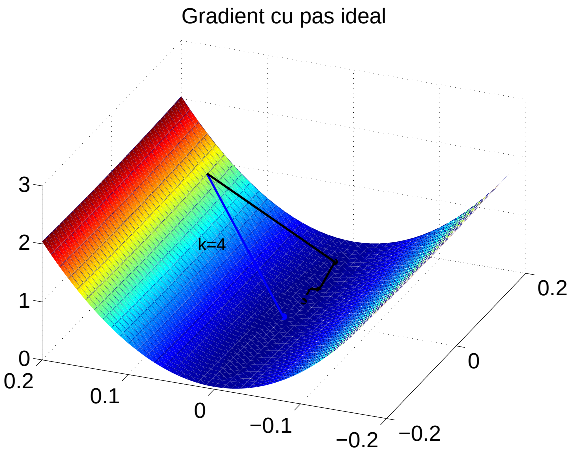


Metoda Newton versus metoda gradient



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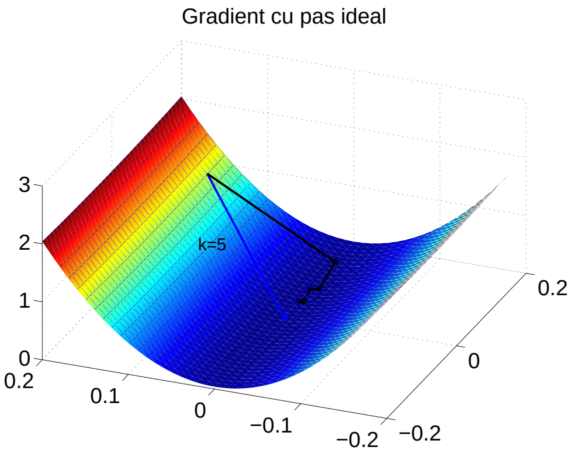

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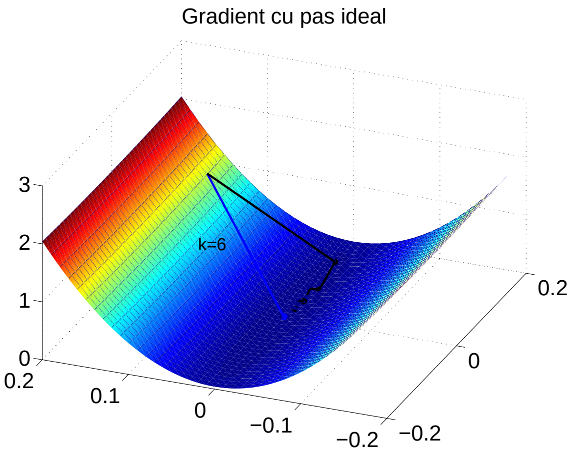
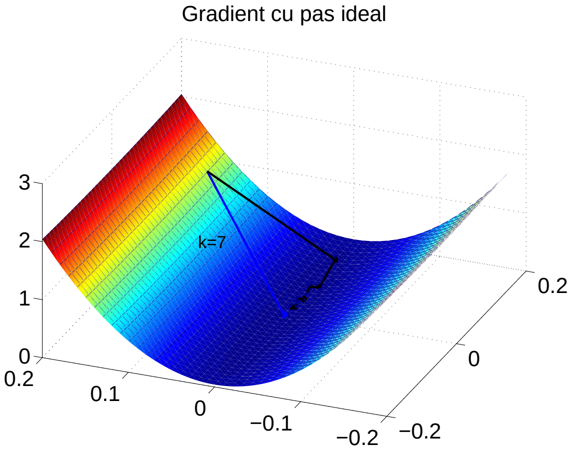


Metoda Newton versus metoda gradient



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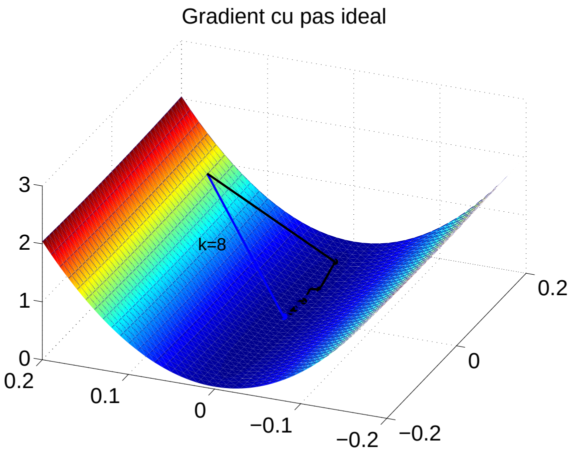
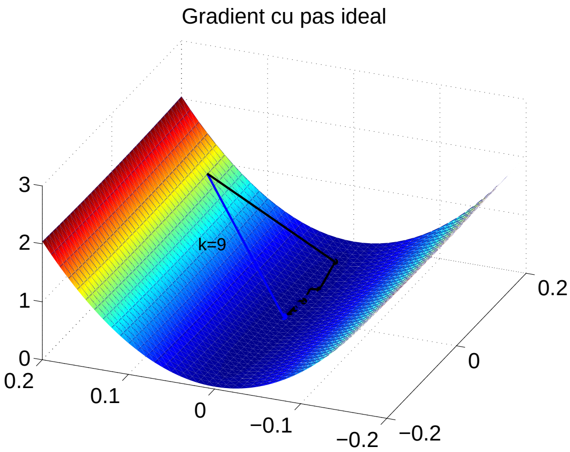


Metoda Newton versus metoda gradient



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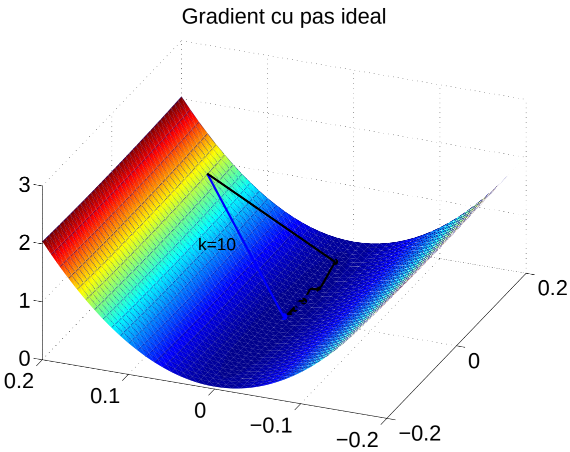
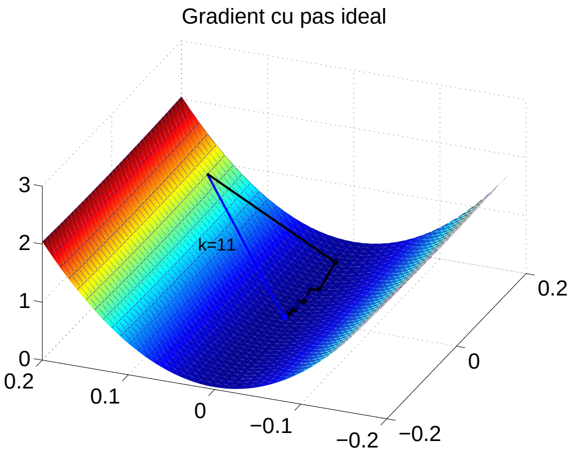
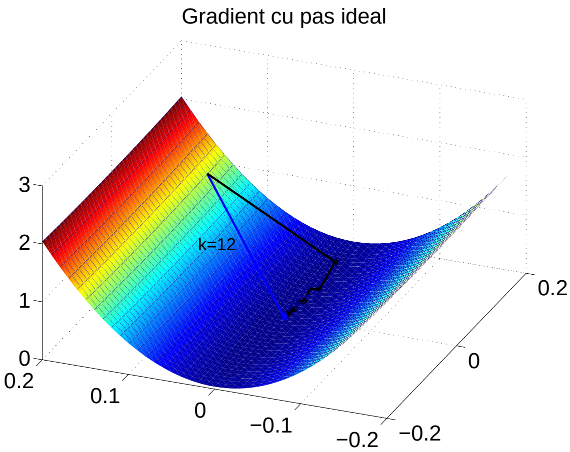


Metoda Newton versus metoda gradient



Metoda Newton versus metoda gradient



Metoda Newton versus metoda gradient