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Solution 4

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Question 1: Conjugate gradient (CG)

Given a matrix $A(n \times n)$ and the cost function $F(u)$ defined as

$$F(x) = \frac{1}{2}x^T A x - x^T b + c$$

a) Show that $\nabla F(x) = Ax - b$

$$\frac{d(x^T A)}{dx} = A^T \implies \nabla F(x) = \frac{1}{2}\left(A^T + A\right)x - b$$

(by product rule of differentiation)

$$A^T = A \implies \frac{1}{2}\left(A^T + A\right)x - b = Ax - b$$

b) For what property of the matrix A is the solution to the problem $\nabla F(x) = 0$ unique ?

The solution is unique for matrix A being symmetric and positive definite i.e. $x^T A x > 0$, for every non-zero vector x.

c) Given

$$A = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} \quad , \quad b = \begin{pmatrix} 2 \\ -8 \end{pmatrix} \quad , \quad c = 0$$

Compute and plot the quadratic form $F(x)$ with $x_1 \in (-4, 6)$ and $x_2 \in (4, -6)$ as both surface and the contour plots.

d) In the previous problem, check if the solution to $\nabla F(x) = 0$ sits at the global minimum in the plot. Also comment on the positive definiteness of A.

The solution to the linear system $Ax = b$ is $x_1 = 2, x_2 = -2$

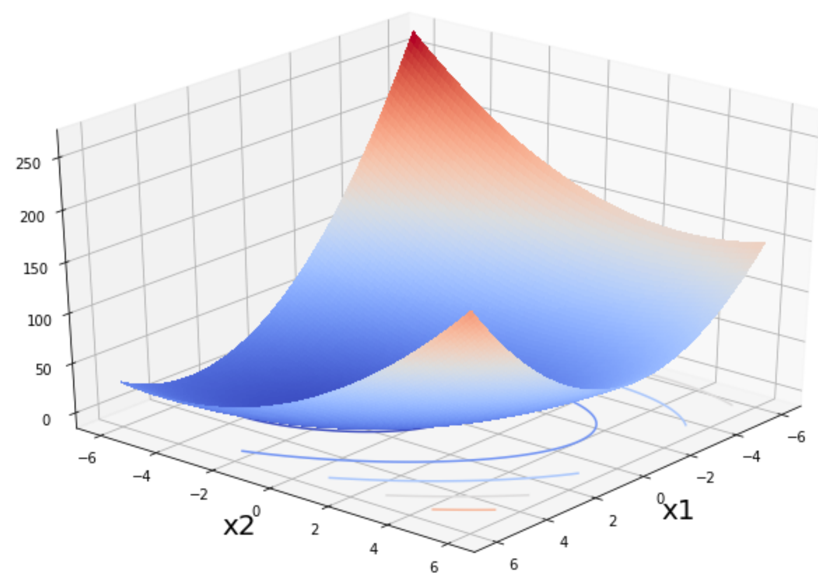

Figure 1: surface plot

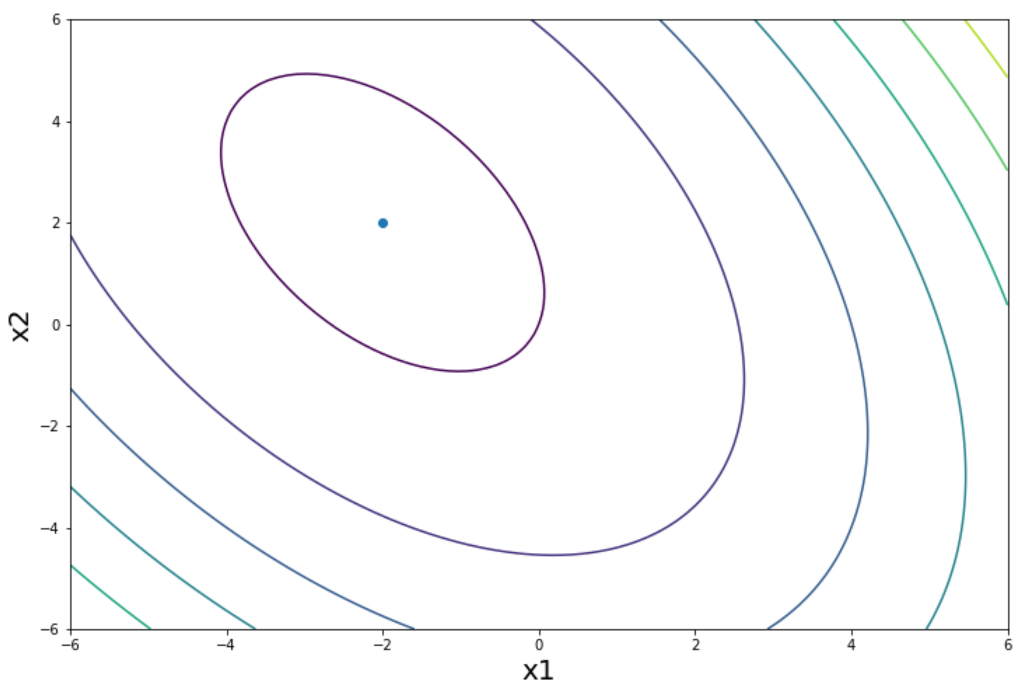

Figure 2: contour plot

Question 2: Convergence analysis of CG method

Given the matrix

$$A = \begin{pmatrix} 3 & 2 & 1 \\ 2 & 3 & 2 \\ 1 & 2 & 3 \end{pmatrix}$$

a) Evaluate the number of iterations required for CG algorithm to reduce the absolute initial error $\|e^0\|_A$ (in the A-norms) by a factor of 10^{-10}.

For conjugate gradient (CG)

$$\|e^k\|_A \leq 2\alpha^k \|e^0\|_A$$

where $\|e^k\|_A = \|u^k - u\|_A$, $\alpha = \frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}$ and $\kappa(A) = \frac{\lambda_{max}(A^TA)}{\lambda_{min}(A^TA)}$

The eigen-values of A^TA are $\lambda_1 = 2, \lambda_2 = 6.37, \lambda_3 = 0.628$.
So the $\kappa(A) = 10.151$ and $\alpha = 0.5222$

Assuming $\|e^0\|_A = 1$,For the initial error $\|e^0\|_A$ to reduce by 10^{-10}, we need $2\alpha^k = 10^{-10}$

$$\begin{aligned} 2\alpha^k &= 10^{-10} \\ k &= \frac{\log(5 \cdot 10^{-11})}{\log(\alpha)} \approx 37 \text{ iterations} \end{aligned}$$

Question 3: Programming task

a) Implement the CG method in MATLAB/python.

b) Test your code for the solution of linear system $Ax = b$ given by,

$$A = \begin{pmatrix} 3 & 1 & 0 & 0 \\ 1 & 4 & 1 & 3 \\ 0 & 1 & 10 & 0 \\ 0 & 3 & 0 & 3 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

c) Compare the solution from your code with MATLAB command `pcg(A,b,tol,maxit)` with `tol` $= 10^{-7}$ and `maxit` $= 1000$. Evaluate the number of iterations and the CPU time required to reach the tolerance `tol`. See if this is consistent with the analysis of the problem 2 a).

d) Repeat b) with the preconditioning Matrix $C = HH^T$, where H is the incomplete Cholesky Decomposition of A. Compare your solution from your code with MATLAB command `pcg(A,b,tol,maxit,M1,M2)`, here `M1` $= H$ and `M2` $= H^T$.
(Hint : Use `ichol(A)` for incomplete Cholesky Decomposition in MATLAB)

e) Given the sparse matrix A ($n \times n$) and the load vector b ($n \times 1$), use your CG algorithm to find the solution of the linear system $Ax = b$ for $n \in (100, 500, 1000, 10000)$ and $h = \frac{1}{n}$.

$$A = \begin{pmatrix} -2 & 1 & 0 & \dots & \dots & \dots & 0 \\ 1 & -2 & 1 & \dots & \dots & \dots & \vdots \\ \vdots & 1 & -2 & 1 & \dots & \dots & \vdots \\ \vdots & \vdots & 1 & -2 & 1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots & 1 & -2 & 1 \\ 0 & 0 & \dots & \dots & 0 & 1 & -2 \end{pmatrix}, \quad b = \begin{pmatrix} 2h^2 \\ 2h^2 \\ 2h^2 \\ \vdots \\ \vdots \\ \vdots \\ 2h^2 \end{pmatrix}$$

f) For the above problem, plot the number of iterations (k), CPU time taken (t) and the condition number (κ) versus the size (n) of the matrix A.

Refer to the following link:
`https://scipy.github.io/old-wiki/pages/ConjugateGradientExample.html`