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Exercise set 5
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Sciences

1 N\&W Exercise 5.4 (p. 133 in 2nd edition). What important condition on the $p$ s is missing in the text? (Hint: Note that you may write $x_{0}+P \sigma$, where $P=$ $\left(p_{0}, p_{1}, \ldots, p_{k-1}\right)$ and $\sigma=\left(\sigma_{0}, \ldots, \sigma_{k-1}\right)^{\mathrm{T}}$.)

## Solution:

In NEW Problem 5.4 (p. 133) we are going to show that if $f(x)$ is a strictly convex, quadratic function, then $h: \mathbb{R}^{k} \rightarrow \mathbb{R}$ defined by $h(\sigma)=f\left(x_{0}+P \sigma\right)$ is also a quadratic and strictly convex function. We know that $f$ is of the form $f(x)=\frac{1}{2} x^{\mathrm{T}} A x-b^{\mathrm{T}} x+a$, where $\nabla^{2} f=A>0$.

We introduce $x_{0}+P \sigma$ in the expression for $f$ :

$$
\begin{aligned}
h(\sigma) & =f\left(x_{0}+\sigma_{0} p_{0}+\cdots+\sigma_{k-1} p_{k-1}\right) \\
& =f\left(x_{0}+P \sigma\right) \\
& =\frac{1}{2}\left(x_{0}+P \sigma\right)^{\mathrm{T}} A\left(x_{0}+P \sigma\right)-b^{\mathrm{T}}\left(x_{0}+P \sigma\right)+a \\
& =\frac{1}{2}\left(x_{0}^{\mathrm{T}} A x_{0}+\sigma^{\mathrm{T}} P^{\mathrm{T}} A x_{0}+x_{0}^{\mathrm{T}} A P \sigma+\sigma^{\mathrm{T}} P^{\mathrm{T}} A P \sigma\right)-b^{\mathrm{T}}\left(x_{0}+P \sigma\right)+a \\
& =\frac{1}{2} \sigma^{\mathrm{T}} P^{\mathrm{T}} A P \sigma+\left(P^{\mathrm{T}} A x_{0}-P^{\mathrm{T}} b\right)^{\mathrm{T}} \sigma+a-b^{\mathrm{T}} x_{0}+\frac{1}{2} x_{0}^{\mathrm{T}} A x_{0} .
\end{aligned}
$$

This is a quadratic function in $\sigma$. Since $A>0, \sigma^{\mathrm{T}} P^{\mathrm{T}} A P \sigma>0$ if and only if $P \sigma \neq 0$. Thus, $P^{\mathrm{T}} A P$ is positive definite (and hence $h$ strictly convex) if and only if $P$ has rank $k$. The missing condition in the problem is that $\left\{p_{k}\right\}$ should be linearly independent. It is probable that $\left\{p_{k}\right\}$ were meant to be $A$-orthogonal, which in turn implies linear independence.

2 In this problem we shall look at some statements you find in textbooks about the CG method.

The following simple Matlab code for the CG method of a quadratic problem is also stated in the note on the Web:

```
ndim = 100; R = randn(ndim);
npot = .1;
A = (R'*R)`npot;
kappa = max(eig(A))/min(eig(A));
xsol = rand(ndim,1); b = A*xsol;
Norm2 = sqrt(xsol'*xsol); NormA = sqrt(xsol'*A*xsol);
x = zeros(size(b)); g = A*x-b; p = -g;
for loop = 1:ndim
    Ap = A*p;
    alfa = - (p'*g)./(p'*Ap);
    x = x + alfa*p;
    g=g + alfa*Ap; % g=A*x-b;
```



Figure 1: Convergence in 2-norm, $A$-norm and the error bound stated in the problem. Size of system $=400$.

```
    beta = (g'*Ap)./ (p'*Ap);
    p = -g + beta*p;
    err2(loop) = sqrt((x-xsol)'*(x-xsol))/Norm2;
    errA(loop) = sqrt((x-xsol)'*A*(x-xsol))/NormA;
end
semilogy(1:ndim, err2,1:ndim,errA,'r');
legend('2-norm', 'A-norm');
xlabel('Iteration
Tittel = ['npot=ड' num2str(npot) 'ப\kappa=',num2str(kappa)];
title(Tittel);
```

a) Implement and plot the error bound

$$
\left\|x_{k}-x^{*}\right\|_{A} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{k}\left\|x_{0}-x^{*}\right\|_{A}
$$

in the Matlab code above. How does this compare with the actual decrease of the error? N\&W say: "This bound often gives a large overestimate". Is this true?
Solution: Before the loop we introduce

```
errBound= (sqrt(kappa)-1)/(sqrt(kappa)+1);
```

and in the loop the errorbound is computed along with the others:

```
err2(loop) = sqrt((x-xs\circl)'*(x-xs\circl))/Norm2;
errA(loop) = sqrt((x-xs\circl)'*A*(x-xs\circl))/NormA;
errB(loop) = 2*(errBound^loop)*NormA;
```

One example is shown in Fig. 1. Conclusions are left to the investigator!
b) Modify the well-conditioned matrix $A$ so that it has $m$ large eigenvalues $(3 \leq$ $m \leq 6$ ) by adding a random rank- $m$ matrix $L L^{\mathrm{T}}$,

$$
A=\left(R^{\mathrm{T}} R\right)^{\mathrm{npot}}+\mu L L^{\mathrm{T}}, \quad \mu \gg 1
$$

where $L$ is $n \times m$ and consists of just $m$ random column vectors. Test the performance of the CG method in this case.

Hint: Read about this in N\&W p. 115-117 and the note on the web page.

## Solution:

The matrix is generated simply as

```
ndim = 100; R= randn(ndim);
npot = 0.1;
mu = 100; % much larger than 1
L = randn(ndim,5);
A = (R'** ) n npot + mu*L*L';
```

An example is shown in Fig. 2.


Figure 2: Convergence for a $400 \times 400$ matrix where the eigenvalues are clustered: All except 5 are clustered around 1 , and the largerst 5 are about $5 \times 10^{5}$.
c) It is stated in the classic book by Luenberger (and also reproduced in the note) that in case b) above, the CG method should be restarted with a SD step every $m$-th step. Is this really necessary? (The SD step is obtained by setting $\beta=0$ every $m$-th step).

Solution: Try yourself!

