Matrices, moments and quadrature

Gérard MEURANT

September 2009

$[a, b]$ = finite or infinite interval of the real line

We will use Riemann–Stieltjes integrals of a real valued function f of a real variable with respect to a real function α which are denoted by

$$\int_a^b f(\lambda)\, d\alpha(\lambda) \tag{1}$$

In many cases Riemann–Stieltjes integrals are directly written as

$$\int_a^b f(\lambda)\, w(\lambda) d\lambda$$

where w is called the weight function

Moments

Let α be a nondecreasing function on the interval (a, b) having finite limits at $\pm\infty$ if $a = -\infty$ and/or $b = +\infty$

Definition

The numbers

$$\mu_i = \int_a^b \lambda^i \, d\alpha(\lambda), \ \ i = 0, 1, \ldots \tag{2}$$

are called the **moments** related to the measure α

A little bit of history 1

Famous names are associated with moment problems : Chebyshev, Markov, Stieltjes, Hamburger, Hausdorff

In 1894–1895, Stieltjes published a seminal paper : "Recherches sur les fractions continues" Ann. Fac. Sci. Toulouse, v 8, (1894), J1–122, v 9 , (1895)

He proposed and solved the following problem :
Find a bounded non–increasing function α in the interval $[0, \infty)$ such that its moments have a prescribed set of values μ_n

$$\int_0^{\infty} \lambda^n \, d\alpha(\lambda) = \mu_n, \;\; n = 0, 1, 2, \ldots$$

The name "problem of moments" was chosen by Stieltjes in analogy with mechanical problems

A little bit of history 2

see the books by

Shohat and Tamarkin

The problem of moments, American Mathematical Society, (1943)

and

Akhiezer

The classical moment problem, Oliver and Boyd, London (1965).
Russian edition 1961

A little bit of history 3

Moment problems in numerical linear algebra (related to the estimation of error norms) :

G. Dahlquist, S.C. Eisenstat and G.H. Golub,
Bounds for the error of linear systems of equations using the theory of moments,
J. Math. Anal. Appl., v 37, (1972), pp 151–166

G. Dahlquist, G.H. Golub and S.G. Nash,
Bounds for the error in linear systems.
In Proc. of the Workshop on Semi–Infinite Programming, R. Hettich Ed., Springer (1978), pp 154–172

The first paper considers a sequence of Krylov vectors $r^{i+1} = Ar^i$, $i = 0, 1, \dots k-1$ (this may not be such a good idea numerically) and looks at the moments

$$(r^i, r^j) = (A^{i+j} r^0, r^0) = \mu_{i+j}$$

Assume A is SPD, given μ_i, $i = 0, \dots, 2k$ how do we compute bounds for $\mu_{-2} = (A^{-2} r^0, r^0)$?

We will see in a moment why they were interested in that problem

In these 2 papers, the authors used beautiful relationships between matrices, moments, orthogonal polynomials, quadrature, ...

Examples of applications 1

Solve

$$Ax = b$$

Let x^k be an approximate solution and $r^k = b - Ax^k$ be the residual vector

Since $\|r^k\|$ is often misleading for stopping iterative methods, it is of interest to obtain bounds or estimates of norms of the error

$$\epsilon^k = x - x^k$$

We have

$$A\epsilon^k = r^k$$

Therefore,

$$\|\epsilon^k\|_A^2 = (A\epsilon^k, \epsilon^k) = (A^{-1}r^k, r^k) = (r^k)^T A^{-1} r^k \ (A \text{ SPD})$$

$$\|\epsilon^k\|^2 = (r^k)^T A^{-2} r^k$$

We have to consider quadratic forms $u^T f(A) u$ with $u = r^k$ and $f(x) = 1/x$ or $1/x^2$

Examples of applications 2

Ill-posed problems

We want to solve

$$Ax = y$$

where A ($m \times n$ matrix) arises from the discretization of an inverse problem (Fredholm integral equation of the first kind)

Generally, the right hand side is corrupted with (an unknown) noise

$$y = \hat{y} + e$$

The matrix A may have very small singular values

Tikhonov regularization

$$(A^T A + \nu I)x = A^T y$$

How to choose the regularization parameter ν ?

Generalized Cross Validation (GCV) :
see G.H. Golub, M. Heath and G. Wahba (1979)
find the minimum of

$$G(\nu) = \frac{\frac{1}{m}\|(I - A(A^TA + \nu I)^{-1}A^T)y\|^2}{(\frac{1}{m}\mathrm{tr}(I - A(A^TA + \nu I)^{-1}A^T))^2}$$

L-curve : find the "corner" of $\log(\|x(\nu)\|)$ as a function of $\log(\|y - Ax(\nu)\|)$

Easy to solve if we know the SVD of A, not feasible if the matrix is large

In these methods and others we need to compute

$$y^T A (A^T A + \nu I)^{-p} A^T y$$

and/or

$$y^T (A A^T + \nu I)^{-p} y$$

$p = 1, 2, 3, 4,\;$ for given ν and y

Examples of applications 3

Total least squares (TLS)
see G.H. Golub and C. Van Loan (1980)

We look for the solution of

$$\min_{E,r} \|(E, r)\|_F$$

subject to

$$(A + E)x = b + r, \quad A : m \times n$$

The minimum is given by σ_{n+1} (the smallest singular value of $\begin{pmatrix} A & b \end{pmatrix}$) which is the solution of the secular equation

$$\sigma_{n+1}^2 = b^T b - b^T A (A^T A - \sigma_{n+1}^2 I)^{-1} A^T b$$

This is the same type of function as in GCV

Other examples

Rank one change for eigenvalues

$$Ax = \lambda x, \quad (A + c^T c)y = \mu y$$

Secular equation :

$$1 + c^T (A - \mu I)^{-1} c = 0$$

Quadratic constraint

$$A = A^T, \quad \min_x x^T Ax - 2b^T x, \; x^T x = \alpha^2$$

Secular equation :

$$b^T (A - \mu I)^{-2} b = \alpha^2$$

Relation to quadrature

Assume A is symmetric positive definite

$$A = Q\Lambda Q^T, \quad Q^T Q = I$$

Λ diagonal

Consider

$$u^T f(A) u, \quad f(A) = Q f(\Lambda) Q^T$$

We write the quadratic form as a Riemann–Stieltjes integral

$$I[f] = u^T f(A) u = \int_a^b f(\lambda)\, d\alpha(\lambda)$$

the measure α is piecewise constant
if $y = Q^T u$

$$\alpha(\lambda) = \begin{cases} 0 & \text{if } \lambda < a = \lambda_1, \\ \sum_{j=1}^{i} y_j^2 & \text{if } \lambda_i \leq \lambda < \lambda_{i+1}, \\ \sum_{j=1}^{n} y_j^2 & \text{if } b = \lambda_n \leq \lambda \end{cases}$$

λ_i are the eigenvalues of A that we usually don't know

We would like to approximate or to bound the integral by using Gauss quadrature rules

Gauss quadrature

$$I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda) = \sum_{j=1}^{N} w_j f(t_j) + \sum_{k=1}^{M} v_k f(z_k) + R[f]$$

the weights $[w_j]_{j=1}^N, [v_k]_{k=1}^M$ and the nodes $[t_j]_{j=1}^N$ are unknowns and the nodes $[z_k]_{k=1}^M$ are prescribed

$$R[f] = \frac{f^{(2N+M)}(\eta)}{(2N+M)!} \int_a^b \prod_{k=1}^{M} (\lambda - z_k) \left[\prod_{j=1}^{N} (\lambda - t_j) \right]^2 d\alpha(\lambda)$$

$$a < \eta < b$$

What is important is the sign of the remainder

Gauss rule : $M = 0$ no prescribed nodes

Suppose $f^{(2n)}(\xi) > 0, \ \forall n, \ \forall \xi, \ a < \xi < b$, then

$$L_G[f] = \sum_{j=1}^{N} w_j^G f(t_j^G)$$

$$L_G[f] \leq I[f]$$

Gauss–Radau rule : $M = 1$ (one node is prescribed), $z_1 = a$ or $z_1 = b$

Suppose $f^{(2n+1)}(\xi) < 0$, $\forall n$, $\forall \xi, a < \xi < b$, then

$$U_{GR}[f] = \sum_{j=1}^{N} w_j^a f(t_j^a) + v_1^a f(a), \quad z_1 = a$$

$$L_{GR}[f] = \sum_{j=1}^{N} w_j^b f(t_j^b) + v_1^b f(b), \quad z_1 = b$$

$$L_{GR}[f] \le I[f] \le U_{GR}[f],$$

Gauss–Lobatto rule : $M = 2$ (two nodes are prescribed), $z_1 = a, z_2 = b$

Suppose $f^{(2n)}(\xi) > 0,\ \forall n,\ \ \forall \xi, a < \xi < b$, then

$$U_{GL}[f] = \sum_{j=1}^{N} w_j^{GL} f(t_j^{GL}) + v_1 f(a) + v_2 f(b)$$

$$I[f] \leq U_{GL}[f],$$

Computation of nodes and weights

Relation to orthogonal polynomials, see G.H. Golub and J.H. Welsch (1969)

$$\int_a^b p_i(\lambda)p_j(\lambda)\; d\alpha(\lambda) = \begin{cases} 1 & \textit{if } \text{i=j} \\ 0 & \textit{otherwise} \end{cases}$$

They satisfy a three–term recurrence

$$\gamma_j p_j(\lambda) = (\lambda - \omega_j)p_{j-1}(\lambda) - \gamma_{j-1}p_{j-2}(\lambda), \quad j = 1, 2, \ldots, N$$

In matrix form

$$\lambda P(\lambda) = J_N P(\lambda) + \gamma_N p_N(\lambda) e_N$$

$$P(\lambda)^T = [p_0(\lambda) \; p_1(\lambda) \cdots \; p_{N-1}(\lambda)]$$

$$J_N = \begin{pmatrix} \omega_1 & \gamma_1 & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_{N-2} & \omega_{N-1} & \gamma_{N-1} \\ & & & \gamma_{N-1} & \omega_N \end{pmatrix}$$

The nodes of the Gauss rule are the eigenvalues of J_N and the weights are the squares of the first elements of the normalized eigenvectors

To obtain the Gauss–Radau rule ($M = 1$), we extend the matrix J_N such that it has one prescribed eigenvalue (a or b)

This is an inverse eigenvalue problem, see G.H. Golub (1973)

$$\hat{J}_{N+1} = \begin{pmatrix} J_N & \gamma_N e_N \\ \gamma_N (e_N)^T & \omega_{N+1} \end{pmatrix}$$

We compute ω_{N+1} by

$$\omega_{N+1} = a - \gamma_N \frac{p_{N-1}(a)}{p_N(a)}$$

$$(J_N - aI)\delta(a) = \gamma_N^2 e_N, \quad \omega_{N+1} = a + \delta_N(a)$$

We do something similar for Gauss–Lobatto

$$(J_N - aI)\delta = e_N, \quad (J_N - bI)\mu = e_N$$

$$\begin{pmatrix} 1 & -\delta_N \\ 1 & -\mu_N \end{pmatrix} \begin{pmatrix} \omega_{N+1} \\ \gamma_N^2 \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

We can compute the nodes and weights by using Golub and Welsch, but this is not always necessary

We have

$$\sum_{l=1}^{N} w_l f(t_l) = (e_1)^T f(J_N) e_1$$

e_1 is the first column of the identity matrix
Sometimes, we can compute the (1,1) element of $f(J_N)$ efficiently (example : $f(x) = 1/x$)

Computation of the orthogonal polynomials

Suppose $\|u\| = 1$ then the matrix J_N is computed by N iterations of the Lanczos algorithm starting from $v^1 = u$

$$\gamma_k = \|\tilde{v}^k\|,$$

$$v^k = \frac{\tilde{v}^k}{\eta_k},$$

$$\omega_k = (v^k, Av^k) = (v^k)^T Av^k,$$

$$\tilde{v}^{k+1} = Av^k - \omega_k v^k - \gamma_k v^{k-1}.$$

The algorithm to compute bounds of $u^T f(A)u$

Suppose the derivatives of f have constant signs, then

- do Lanczos iterations from $u/\|u\|$ to compute J_i
- compute $e_1^T f(J_i)e_1$ or $e_1^T f(\hat{J}_i)e_1$ to obtain bounds

or compute the eigenvalues and (first components of) eigenvectors of J_i

Bilinear forms

To estimate $u^T f(A) v$ when $u \neq v$ we can use

- $u^T f(A) v = [(u+v)^T f(A)(u+v) - (u-v)^T f(A)(u-v)]/4$
- the non-symmetric Lanczos algorithm
- the block Lanczos algorithm

see G.H. Golub and G. Meurant (1994)

Reprinted in

Milestones in Matrix Computations, the selected works of Gene H. Golub with commentaries, R.H. Chan, C. Greif and D.P. O'Leary Eds, Oxford University Press, (2007)

The conjugate gradient algorithm

What to do for CG ?

It does not make sense to do Lanczos iterations starting from $r^k/\|r^k\|$

However, since $A\epsilon^k = r^k = r^0 - AV_k y^k$ and $J_k y^k = \|r^0\|^2 e^1$

$$\|\epsilon^k\|_A^2 = \|r^0\|^2[(J_n^{-1}e^1, e^1) - (J_k^{-1}e^1, e^1)]$$

Note that $\|r^0\|^2(J_n^{-1}e^1, e^1) = (A^{-1}r^0, r^0)$

Hence, $\|\epsilon^k\|_A^2$ is the remainder of Gauss quadrature for the Riemann–Stieltjes integral $(A^{-1}r^0, r^0)$

$$\|\epsilon^k\|_A^2 = \frac{1}{\xi_k^{2k+1}} \sum_{i=1}^{n} \left[\prod_{j=1}^{k} (\lambda_i - \theta_j^{(k)})^2 \right] (r^0, q^i)^2,$$

where q^i is the ith eigenvector of A corresponding to λ_i, $\theta_j^{(k)}$ Ritz values (eigenvalues of J_k), $a \le \xi \le b$

The formula for $\|\epsilon^k\|_A^2$ is equivalent to a formula proved in Hestenes and Stiefel (1952)

$$\|\epsilon^k\|_A^2 = \sum_{j=k}^{n-1} \gamma_j \|r^k\|^2$$

γ_j is one of the two CG parameters

Approximation of the norm of the error

Of course, we do not know $(J_n^{-1}e^1, e^1)$

Let d be a positive integer, at iteration k we use

$$\|\epsilon^{k-d}\|_A^2 \simeq \|r^0\|^2[(J_k^{-1}e^1, e^1) - (J_{k-d}^{-1}e^1, e^1)]$$

or

$$\|\epsilon^{k-d}\|_A^2 \simeq \sum_{j=k-d+1}^{k} \gamma_j \|r^k\|^2$$

The first formula can also be used with Gauss–Radau or Gauss–Lobatto rules to obtain upper bounds

If we want a lower bound for $\|e^{k-d}\|_A^2$ we use the H-S formula

If we have an estimate of the smallest eigenvalue, we compute $(\hat{J}_k^{-1})_{1,1}$ incrementally by using the Sherman–Morrison formula to obtain an upper bound, see Meurant (1997, 1999)

Strakoš and Tichý (2002) have proved that these formulas work also in finite precision arithmetic

Arioli (2004) and Arioli, Loghin and Wathen (2005) have used these techniques to provide reliable stopping criteria for finite element problems

Elements of $f(A)$

Finite difference approximation of the Poisson equation on a 16×16 mesh ($n = 256$)
We look for $(A^{-1})_{125,125}$ whose value is 0.5604

rule	Nit=2	4	6	8	10	20
G	0.3333	0.4337	0.4920	0.5201	0.5378	0.5600
G–R b_L	0.3639	0.4514	0.5006	0.5255	0.5414	0.5601
G–R b_U	1.5208	0.8154	0.6518	0.5925	0.5730	0.5604
G–L	2.1011	0.8983	0.6803	0.6012	0.5760	0.5604

Block Lanczos, $m = 6, n = 36$

$(A^{-1})_{2,1} = 0.1040$

rule	Nit=2	4	6	8
G	0.0894	0.1008	0.1033	0.1040
G–R b_L	0.0931	0.1017	0.1035	0.1040
G–R b_U	0.1257	0.1059	0.1042	0.1040
G–L	0.1600	0.1079	0.1041	0.1041

Larger example

Block Lanczos, $m = 30$, $n = 900$

$(A^{-1})_{1,1} = 0.302346$, $(A^{-1})_{2,2} = 0.344408$, $(A^{-1})_{2,1} = 0.104693$

Results after 10 block iterations for Gauss :

$$\begin{pmatrix} 0.3021799137963044 & 0.1043616568803480 \\ 0.1043616568803480 & 0.3437475221129595 \end{pmatrix}$$

Results after 10 block iterations for Gauss–Radau with exact eigenvalues :

$$\begin{pmatrix} 0.3022010722636479 & 0.1044036770842950 \\ 0.1.044036770842950 & 0.3438314340061286 \end{pmatrix}$$

$$\begin{pmatrix} 0.3039414302035057 & 0.1078375193911064 \\ 0.1078375193911064 & 0.3506698361080970 \end{pmatrix}$$

Exponential of A

Finite difference approximation of the Poisson equation on a 30×30 mesh

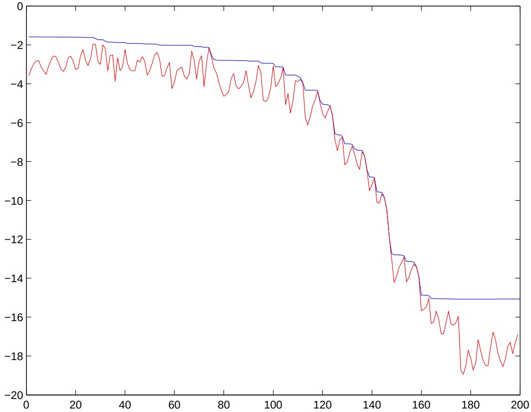
We look for $(exp(A))_{18,18}$ whose value is 197.9724768113708 using Gauss quadrature

After 5 iterations : 197.9|599617609761

After 10 iterations : 197.9724768113|530

CG error norm

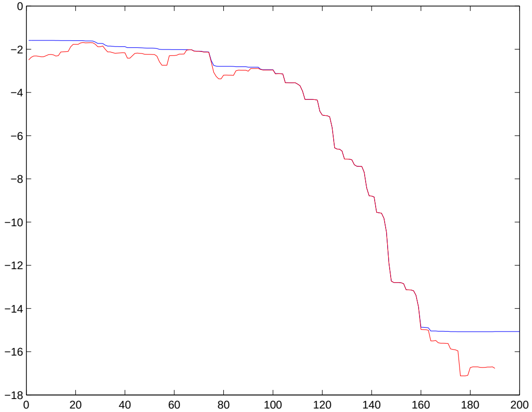
Matrix Bcsstk01, $n = 48$



A norm (blue), Gauss quad $d = 1$ (red)

CG error norm 2

Matrix Bcsstk01, $n = 48$

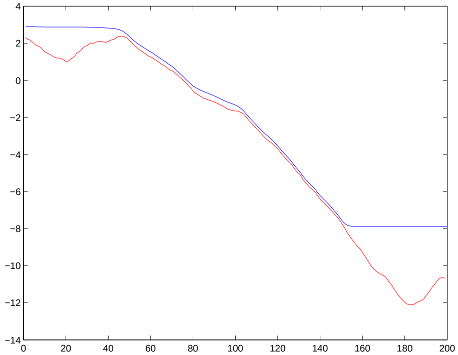


A norm (blue), Gauss quad $d = 10$ (red)

PCG error norm

Elliptic problem, diff. coeff.$= \frac{1}{(2+p\sin\frac{x}{\eta})(2+p\sin\frac{y}{\eta})}$

$p = 1.99$ and $\eta = 0.01$, mesh 100×100, IC(0)



A norm (blue), Gauss quad $d = 1$ (red)

Ill–posed problems (Tikhonov using GCV)

The matrix to consider is $B = A^T A$ or $B = AA^T$

We use the Golub–Kahan bidiagonalization algorithm (1965) which produces a lower bidiagonal matrix C_k

We have to compute quantities like

$$I[C_k] = (e^1)^T (C_k^T C_k + \nu I)^{-p} e^1$$

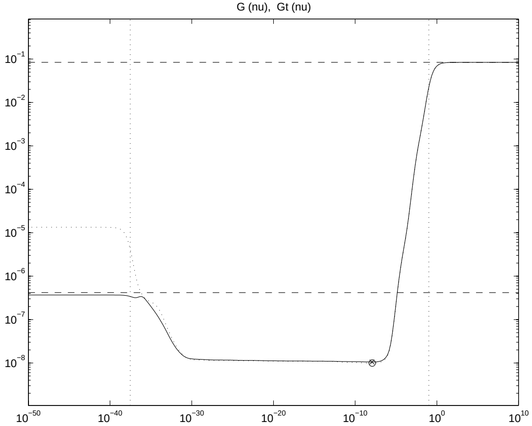
This can be done by solving least squares problems or by using the SVD of C_k

For computing the trace we use a result of Hutchinson (1989)

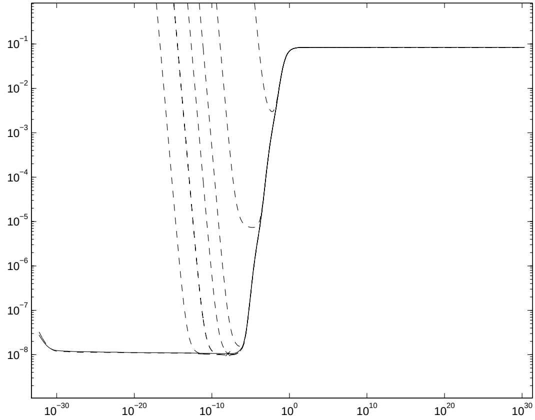
$$tr[(AA^T + \nu I)^{-1}] \approx \frac{1}{q} \sum_{i=1}^{q} (u^i)^T (AA^T + \nu I)^{-1} u^i$$

where u^i are random vectors. In practice, $q = 1$

Problem : Baart, Regutools (Hansen), $n = 100$



functions G and $\tilde{G}$, `Baart`, $m = n = 100$, $\|e\| = 10^{-3}$



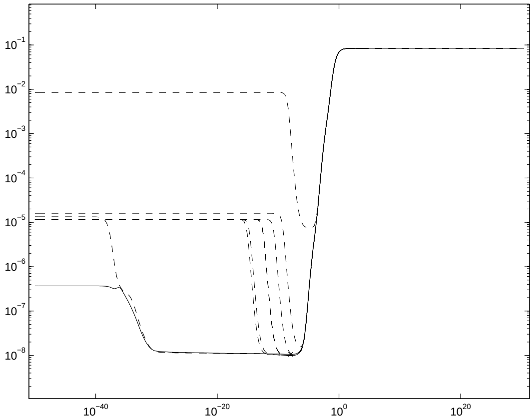
functions G, $\tilde{G}$ and upper bound, `Baart`, $m = n = 100, \|e\| = 10^{-3}$

Notice that

- We do not want to compute the bounds for too many points ν_i
- It would be nice to know that the upper bound has "converged" before looking for the minimum
- The upper bound does not have the right asymptotic behavior when $\nu \to 0$

We modify the function for the upper bound, instead of $p(\nu)/q(\nu)^2$, we consider

$$\frac{p(\nu)}{q(\nu)^2 + \|y\|^2}$$



functions G, $\tilde{G}$ and modified upper bound, `Baart`,
$m = n = 100, \|e\| = 10^{-3}$

- We test the convergence of the upper bounds for a small value of ν
- We compute the minimum
- We test its convergence
- Functions values are computed using SVDs of C_k

Baart

	$\|e\|$	nb it	ν/m	f min
GM	10^{-7}	12	$1.0706\ 10^{-14}$	436
	10^{-5}	12	$1.0581\ 10^{-11}$	437
	10^{-3}	8	$1.3077\ 10^{-8}$	293
	10^{-1}	7	$1.1104\ 10^{-7}$	294
	10	7	$9.1683\ 10^{-8}$	294

ILaplace

	$\|e\|$	nb it	ν/m	f min
GM	10^{-7}	58	$4.2396\ 10^{-14}$	5239
	10^{-5}	28	$5.4552\ 10^{-11}$	1453
	10^{-3}	17	$2.3046\ 10^{-8}$	440
	10^{-1}	15	$2.0896\ 10^{-5}$	293
	10	10	$6.8436\ 10^{-3}$	296

ILaplace

	$\|e\|$	ν/m	$\|y-Ax\|$	$\|x-x_0\|$	t(s)
GM	10^{-7}	$4.2396\ 10^{-14}$	$1.1004\ 10^{-7}$	$2.7130\ 10^{-2}$	2.03
	10^{-5}	$5.4552\ 10^{-11}$	$1.0560\ 10^{-5}$	$9.6771\ 10^{-2}$	0.53
	10^{-3}	$2.3046\ 10^{-8}$	$9.7243\ 10^{-4}$	$1.9937\ 10^{-1}$	0.29
	10^{-1}	$2.0896\ 10^{-5}$	$9.8235\ 10^{-2}$	$3.4634\ 10^{-1}$	0.09
	10	$6.8436\ 10^{-3}$	9.9115	$8.8791\ 10^{-1}$	0.14

x_0 is the noise free exact solution

go to the end

Another application : computing the trace of the inverse

Let A be symmetric (positive definite for the sake of simplicity)

There are applications in physics where it is desired to compute bounds or estimates of the trace of the inverse $tr(A^{-1})$ and/or the determinant $\det(A)$ of large sparse matrices

Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the eigenvalues of A
We have

$$tr(A^r) = \sum_{i=1}^{n} \lambda_i^r$$

We are interested in $r = -1$

As we have seen the sum $\sum_{i=1}^{n} \lambda_i^r$ can be written as a Riemann–Stieltjes integral

$$tr(A^r) = \mu_r = \int_a^b \lambda^r \, d\alpha, \quad a \leq \lambda_1, \; \lambda_n \leq b$$

where the (unknown) measure α is given as

$$\alpha(\lambda) = \sum_{j=1}^{n} H(\lambda - \lambda_j)$$

H is the unit step function, $H(\lambda) = 0, \, \lambda < 0, \; H(\lambda) = 1, \, \lambda \geq 0$

The values μ_r are the moments related to α

We wish to compute

$$\mu_{-1} = \int_a^b \frac{1}{\lambda} \, d\alpha$$

Bai and Golub results

As before use Gauss quadrature to estimate or bound the integral

Bai and Golub (1997) use three moments $r = 0, 1, 2$

$$\mu_0 = n, \quad \mu_1 = \mathrm{tr}(A) = \sum_{i=1}^{n} a_{i,i}, \quad \mu_2 = \mathrm{tr}(A^2) = \sum_{i,j=1}^{n} a_{i,j}^2 = \|A\|_F^2$$

to analytically compute the nodes and weights of a Gauss–Radau rule and then bounds for the integral of $1/\lambda$

Bai and Golub results 2

Their result is

$$\begin{pmatrix}\mu_1 & n\end{pmatrix}\begin{pmatrix}\mu_2 & \mu_1\\ b^2 & b\end{pmatrix}^{-1}\begin{pmatrix}n\\ 1\end{pmatrix} \le \mathrm{tr}(A^{-1}) \le \begin{pmatrix}\mu_1 & n\end{pmatrix}\begin{pmatrix}\mu_2 & \mu_1\\ a^2 & a\end{pmatrix}^{-1}\begin{pmatrix}n\\ 1\end{pmatrix}$$

This result is nice since the moments $\mu_0,\ \mu_1,\ \mu_2$ are easy to compute, but in many cases, the bounds are far from being sharp

Associated with the measure α there exist orthonormal polynomials p_k

They satisfy a three-term recurrence

$$\gamma_j p_j(\lambda) = (\lambda - \omega_j) p_{j-1}(\lambda) - \gamma_{j-1} p_{j-2}(\lambda), \quad j = 1, 2, \ldots, n$$

The Jacobi matrix is

$$J_k = \begin{pmatrix} \omega_1 & \gamma_1 & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_{k-2} & \omega_{k-1} & \gamma_{k-1} \\ & & & \gamma_{n-1} & \omega_k \end{pmatrix}$$

The main question is :

Can we compute the Jacobi matrix from the moments ?

If we can do this, we have the algorithm :

moments ($r \geq 0$) $\Rightarrow$ Jacobi matrix $\Rightarrow$ eigensystem $\Rightarrow$ nodes and weights $\Rightarrow$ estimate for $r = -1$

The Chebyshev algorithm

An answer to our question has been given by Chebyshev (1859) who described an algorithm to obtain the coefficients of the orthogonal polynomials from the moments

One needs $2k$ moments to compute J_k

The algorithm (as it is described today) uses the Cholesky factorization of the (Hankel) moment matrix $m_{i,j} = \mu_{i+j-2}$

However, the map from the moments to the coefficients is ill-conditioned (see Gautschi) and the Chebyshev algorithm is often unstable

The modified Chebyshev algorithm

This algorithm was developed by J. Wheeler in 1974, see also Sack and Donovan (1972)

Let π_k be a family of known orthogonal polynomials satisfying

$$b_{k+1}\pi_{k+1}(\lambda) = (\lambda - a_{k+1})\pi_k(\lambda) - c_k\pi_{k-1}(\lambda)$$

The modified moments are

$$m_l = \int_a^b \pi_l(\lambda)\, d\alpha$$

which have to be known

The algorithm uses mixed moments which are

$$\sigma_{k,l} = \int_a^b p_k(\lambda)\pi_l(\lambda)\, d\alpha(\lambda)$$

Implementation

As auxiliary polynomials, we use the shifted Chebyshev polynomials :

$$C_0(\lambda) \equiv 1, \quad \left(\frac{\lambda_n - \lambda_1}{2}\right) C_1(\lambda) = \lambda - \left(\frac{\lambda_n + \lambda_1}{2}\right)$$

$$\left(\frac{\lambda_n - \lambda_1}{4}\right) C_{k+1}(\lambda) = \left(\lambda - \frac{\lambda_n + \lambda_1}{2}\right) C_k(\lambda) - \left(\frac{\lambda_n - \lambda_1}{4}\right) C_{k-1}(\lambda)$$

Computing the modified moment m_l is computing the trace of the matrix $C_l(A)$

Pb : we have to compute the product of "sparse" matrices, but we have to store only the last 2 of them

Numerical experiments

Example : Poisson equation

$n = 36$, $tr(A^{-1}) = 13.7571$, Bai and Golub bounds

$$10.2830 \leq tr(A^{-1}) \leq 24.3776$$

Moments

k	bound
1	9.0000
2	11.3684
3	12.5714
4	13.1581
5	13.4773
6	13.6363
7	13.7139
8	13.7452
9	13.7550
10	13.7568

After $k = 10$ the moment matrices are no longer positive definite

Modified Moments

k	bound
1	9.0000
2	11.3684
3	12.5714
4	13.1581
5	13.4773
6	13.6363
7	13.7139
8	13.7452
9	13.7550
10	13.7568
11	13.7571

$n = 900$, $tr(A^{-1}) = 512.6442$, Bai and Golub bounds

$$261.003 \leq tr(A^{-1}) \leq 8751.76$$

The Chebyshev algorithm breaks down after $k = 10$

Modified Moments

k	bound
5	400.0648
10	463.2560
15	489.5383
20	502.0008
25	508.0799
30	510.9301
35	512.1385
40	512.5469

- We can avoid computing the matrices $C_l(A)$ and then their traces by using a Monte Carlo technique :
  Use random vectors z whose components are 1 and -1 with probability $1/2$, then $z^T B z$ is an estimator of $tr(B)$
  One just needs to compute $C_l(A)z$ and an inner product
- The same techniques can be used to estimate $\det(A)$ by remarking that $\det(A) = exp[tr(\ln(A))]$

There is a forthcoming book which should appear soon :

G.H. Golub and G. Meurant

Matrices, moments and quadrature with applications

Princeton University Press

for details see http ://pagesperso-orange.fr/gerard.meurant

Gene H. Golub (1932–2007)