

Prescreening of Two-Electron Integral Derivatives in SCF Gradient and Hessian Calculations

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The definition and implementation of a rigorous two-electron integral bound based on Schwarz' inequality both for gradient and hessian calculations is presented. Tests demonstrate the advantages of this easily implemented and effective bound.

INTRODUCTION

The standard formulation of ab initio SCF and (first-order) gradient methods suggests an N^4 dependence of computational effort, where N denotes the number of basis functions employed. The " N^4 law" does not hold, however, for the most important case, a series of molecules with increasing number of atoms and fixed atomic basis sets,¹ e.g., hydrocarbons C_nH_{2n+2} for increasing n . Empirical evidence indicates in fact an N^a dependence with $2 < a \leq 3$ in such a case of extended systems.² Recent applications³ of the SCF method to molecules with about 100 atoms, 1000 basis functions (and ca. 1000 electrons) have been possible only since the N^4 law does not hold.

The evaluation and processing of two-electron integrals clearly constitutes the bottleneck in SCF and gradient calculations, which asymptotically scales roughly with N^2 for sufficiently large molecules.¹ This is a result of the smallness of most two-electron integrals, which allows to skip their evaluation and further processing. This strategy requires a prescreening of integrals to establish if nonnegligible contributions have to be expected and the actual integral has to be evaluated. The following bound⁴⁻⁶ (which is just a special case of the Schwarz inequality) has proved useful for this purpose

$$|(v\mu|\chi\lambda)| \leq Q_{v\mu}Q_{\chi\lambda} \quad (1)$$

where for (basis) functions f_v

$$(v\mu|\chi\lambda) = \int f_v(r)f_\mu(r)|r-s|^{-1}f_\chi(s)f_\lambda(s) d\tau \quad (2)$$

$$Q_{v\mu} = [(v\mu|v\mu)]^{1/2} \quad (3)$$

The bound (eq. (1)) has two important advantages: it is rigorous for arbitrary f_v and it involves only the two-index quantities $Q_{v\mu}$, which are easily precom-

puted and stored. It has to be noted that $(v\mu|v\mu)$ in eq. (3) must be evaluated to much higher precision than in usual two-electron integral evaluations; an integral neglecting threshold of about 10^{-30} has proved to be sufficient. Since the equality sign in (1) holds for $(v\mu) = (\chi\lambda)$, the bound cannot be improved without further assumptions. Careful tests have demonstrated that (1) is even relatively sharp.⁶

In the present article we propose a method to exploit the bound (1) in SCF first- and second-derivatives calculations (next section) and report results of test calculations showing the advantage of (1) in the third section.

BOUNDS FOR INTEGRAL DERIVATIVES AND THEIR USE IN GRADIENT AND HESSIAN CALCULATIONS

We consider only the computationally most demanding contributions, E^i and E^{ij} to the first and second derivatives of the SCF energy that involve the differentiated two-electron integrals

$$E^i = \sum_{v\mu\chi\lambda} E^i_{v\mu\chi\lambda} \quad (4a)$$

$$E^i_{v\mu\chi\lambda} = (v\mu|\chi\lambda)^i [4D_{v\mu}D_{\chi\lambda} - D_{v\chi}D_{\mu\lambda} - D_{v\lambda}D_{\mu\chi}] \quad (5a)$$

for the first-order gradient and

$$E^{ij} = \sum_{v\mu\chi\lambda} E^{ij}_{v\mu\chi\lambda} \quad (4b)$$

$$E^{ij}_{v\mu\chi\lambda} = (v\mu|\chi\lambda)^{ij} [4D_{v\mu}D_{\chi\lambda} - D_{v\chi}D_{\mu\lambda} - D_{v\lambda}D_{\mu\chi}] \quad (5b)$$

for the Hessian. For the calculation of second derivatives of the energy with respect to the nuclear coordinates one also needs the derivative Fock matrices

$$F^i_{v\mu} = \sum_{\chi,\lambda} 2(v\mu|\chi\lambda)^i D_{\chi\lambda} - \sum_{\chi,\lambda} (v\chi|\mu\lambda)^i D_{\chi\lambda} \quad (6)$$

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The upper indices i, j in (4), (5), and (6) indicate differentiation of the corresponding quantities with respect to the i th/ j th component ($i = x, y, z, j = x', y', z'$) of a nuclear coordinate, and $D_{\nu\mu}$ denotes elements of the one-particle density.

Since

$$(v\mu|\chi\lambda)^i = (v^i\mu|\chi\lambda) + (v\mu^i|\chi\lambda) + (v\mu|\chi^i\lambda) + (v\mu|\chi\lambda^i) \quad (7a)$$

and

$$(v\mu|\chi\lambda)^{ij} = (v^{ij}\mu|\chi\lambda) + (v^i\mu^j|\chi\lambda) + \dots \quad (7b)$$

we are lead to consider expressions $(v^i\mu|\chi\lambda)$, $(v^i\mu^j|\chi\lambda)$ etc. The bound (1) holds for arbitrary functions—including v^i and v^{ij} etc.—and thus gives

$$|(v^i\mu|\chi\lambda)| \leq Q_{v^i\mu} Q_{\chi\lambda} \quad (8a)$$

$$Q_{v^i\mu} = [(v^i\mu|v^i\mu)]^{1/2} \quad (9a)$$

for first derivatives of integrals and, analogously,

$$|(v^i\mu^j|\chi\lambda)| \leq Q_{v^i\mu^j} Q_{\chi\lambda} \quad (8b)$$

$$Q_{v^i\mu^j} = [(v^i\mu^j|v^i\mu^j)]^{1/2} \quad (9b)$$

as an example for a second derivative of an integral.

Since modern algorithms to evaluate (4) and (5) are batch oriented (integrals $(v\mu|\chi\lambda)$ and/or their derivatives are computed together for all components of shells N, M, K, L) and since derivatives for $i, j = x, y, z$ are consequently obtained together, we define

$$Q_{NM} = \max_{\substack{v \in N \\ \mu \in M}} Q_{v\mu} \quad (10)$$

$$R_{NM} = \max_{\substack{v \in N \\ \mu \in M \\ \text{all } i}} [Q_{v^i\mu} + Q_{v\mu^i}] \quad (11)$$

$$S_{NM} = \max_{\substack{v \in N \\ \mu \in M \\ i \in x, y, z \\ j \in x', y', z'}} [Q_{v^{ij}\mu} + Q_{v^i\mu^j} + Q_{v^j\mu^i} + Q_{v\mu^{ij}}] \quad (12)$$

In an analogous way we define

$$D_{NM} = \max_{\substack{v \in N \\ \mu \in M}} |D_{v\mu}| \quad (13)$$

$$D_{NM, KL} = 4D_{NM}D_{KL} + D_{NK}D_{ML} + D_{NL}D_{MK} \quad (14)$$

For the prescreening of contributions to derivative Fock matrices one needs

$$\tilde{D}_{NM, KL} = \max\{D_{KL}, D_{NM}, 1/4 D_{KM}, 1/4 D_{LM}, 1/4 D_{KN}, 1/4 D_{LN}\} \quad (15)$$

Prescreening of small contributions further requires the following definitions

$$Q = \max_{N, M} Q_{NM} \quad (16)$$

$$R = \max_{N, M} R_{NM} \quad (17)$$

$$S = \max_{N, M} S_{NM} \quad (18)$$

$$D = \max_{N, M, K, L} D_{NM, KL} = 6 \max_{N, M} D_{NM}^2 \quad (19)$$

$$\tilde{D} = \max \tilde{D}_{NM, KL} \quad (20)$$

These definitions yield immediately, for $E_{v\mu, \chi\lambda}^i$ defined in eq. (5a),

$$|E_{v\mu, \chi\lambda}^i| \leq (Q_{NM}R_{KL} + Q_{KL}R_{NM})D_{NM, KL} \quad (21a)$$

and

$$|E_{v\mu, \chi\lambda}^{ij}| \leq (Q_{NM}S_{KL} + Q_{KL}S_{NM} + 2R_{NM}R_{KL})D_{NM, KL} \quad (21b)$$

for $E_{v\mu, \chi\lambda}^{ij}$ defined in eq. (5b).

On the basis of eqs. (21a) and (21b) it is then an easy matter to skip the evaluation of all contributions to E^i and E^{ij} , eqs. (4a), (4b), (5a), and (5b), which contribute less than a chosen threshold \mathfrak{J} . To reduce organizational overhead one can consistently skip entire inner loops over shells if no contribution exceeding \mathfrak{J} arises. A convenient strategy for this purpose is sketched in the two charts.

Loop Structure and Tests on Near Zeros for the Evaluation of E^i Eq. (4a)

N, M, K, L denote shells.

Compute auxiliary quantities defined in eqs. (10), (11), (13), (14), (16), (17), (19)

loop N

test on symmetry

loop M

test on symmetry

skip if $(Q_{NM} \cdot R + Q \cdot R_{NM})D < \mathfrak{J}$

loop K

test on symmetry

loop L

skip if $(Q_{NM} \cdot R_{KL} + Q_{KL} \cdot R_{NM})D < \mathfrak{J}$

test on symmetry

compute $D_{NM, KL}$, eq. (14)

skip if $(Q_{NM} \cdot R_{KL} + Q_{KL} \cdot R_{NM})D_{NM, KL} < \mathfrak{J}$

evaluate $E_{v\mu, \chi\lambda}^i$, eq. (4)

next L

next K

next M

next N

Loop Structure and Tests on Near Zeros for the Evaluation of E^{ij} , Eq. (4b)

Compute auxiliary quantities defined in eqs. (10)–(20)

loop N

test on symmetry

loop M

test on symmetry

skip if $(Q_{NM} \cdot S + Q \cdot S_{NM} \cdot 2R_{NM}R)D < \mathfrak{J}$

and $(Q_{NM} \cdot R + Q \cdot R_{NM})D < \mathfrak{J}$

and $(Q_{NM} \cdot R + Q \cdot R_{NM})\tilde{D} < \mathfrak{J}$

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loop K
  test on symmetry
  loop L
    skip if  $(Q_{NM} \cdot S_{KL} + Q_{KL} \cdot S_{NM} + 2R_{NM}R_{KL})D < \mathfrak{J}$ 
    and  $(Q_{NM} \cdot R_{KL} + Q_{KL} \cdot R_{NM})D < \mathfrak{J}$ 
    and  $(Q_{NM} \cdot R_{KL} + Q_{KL} \cdot R_{NM})\tilde{D} < \mathfrak{J}$ 
  test on symmetry
  compute  $D_{NM,KL}$ , eq. (14)
  compute  $\tilde{D}_{NM,KL}$ , eq. (15)
  skip if  $(Q_{NM}S_{KL} + Q_{KL}S_{NM} + 2R_{NM}R_{KL})D_{NM,KL} < \mathfrak{J}$ 
  and  $(Q_{NM}R_{KL} + Q_{KL}R_{NM})D_{NM,KL} < \mathfrak{J}$ 
  and  $(Q_{NM}R_{KL} + Q_{KL}R_{NM})\tilde{D}_{NM,KL} < \mathfrak{J}$ 
  evaluate  $E_{\nu\mu\lambda}^{ij}$ , eq. (4)
  add contributions to  $F_{\nu\mu}^i$ , eq. (6)
  next L
next K
next M
next N

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In the charts we have also indicated where test on symmetry appear appropriate if symmetry is exploited by just processing the “petite liste”.⁷

For the gradient calculations in the next section, the timings were obtained by the direct implementation of the procedure indicated in the first chart. For Hessian calculations, however, this method which we call “global prescreening” leads to only minor reductions in CPU time by about 5%. As discussed below (see explicitly eqs. (22)–(25)), some additional tests are necessary to gain full advantage of our rigorous bound.

It remains to comment briefly on the evaluation of the quantities defined in eqs. 9(a) and 9(b). They introduce integrals like $(v^i\mu|v^i\mu)$ and $(v^i\mu^j|v^i\mu^j)$ etc., which do not occur otherwise in gradient/Hessian calculations. The easiest way to obtain these quantities is numerical differentiation. Careful tests demonstrated that the straightforward method of finite differences provides sufficient accuracy for this purpose. The implementation of the terms necessary for gradients (which require second-order numerical derivatives) is easily done, but we cannot recommend the somewhat awkward implementation of the terms for the Hessian (which require fourth-order numerical derivatives). A better way for this purpose is to modify an existing force-program to calculate the integrals $(v^i\mu|v^i\mu)$ and $(v\mu^i|v\mu^i)$ analytically and to differentiate these integrals numerically.

By testing the bound, we noticed that the method sketched in the two charts, which we will now refer to as global prescreening, works much better for the gradient than for Hessian calculations. The idea of global prescreening is to estimate all batches of integrals and their derivatives occurring in a given shell quadruple without discriminating between the different types of first derivatives (eq. (7a)) and second derivatives (indicated in eq. (7b)). The method of

screening the different types of second derivatives individually immediately before their evaluation is referred to by us as “local prescreening” (first derivatives are treated as in the gradient). As an example, we consider the individual prescreening of integrals $(v^ij\mu|\chi\lambda)$. We define the quantity

$$Z_{NM} = \max_{v \in N, \mu \in M} (Q_{v^ij\mu}, Q_{v\mu^ij}) \quad (22)$$

which is already calculated for the purpose of global prescreening but has now to be stored. With Z_{NM} defined in this way the evaluation of $(v\mu|\chi\lambda)$ is skipped if

$$(v^ij\mu|\chi\lambda) < Z_{NM} * Q_{KL} < \mathfrak{J} \quad (23)$$

To give another example and to show that there are just two extra arrays to be stored, we consider $(v^i\mu^j|\chi\lambda)$. By defining

$$T_{NM} = \max_{v \in N, \mu \in M} (Q_{v^i\mu^j}, Q_{v^j\mu^i}) \quad (24)$$

the evaluation is skipped if

$$(v^i\mu^j|\chi\lambda)D_{\nu\mu,\chi\lambda} < T_{NM} * Q_{KL} * D_{NM,KL} < \mathfrak{J} \quad (25)$$

All appearing integrals can now be estimated in this more individual way. The extra amount of space is negligible. For Hessian calculations, the timings of the next section were obtained by using these refinements.

The importance of neglecting near zero integrals has, of course, been recognized and exploited in virtually all Quantum Chemistry codes. For the most important case of Gaussian type basis functions this is usually done in the following way. The two-electron integral $(\rho\sigma|\tau\omega)$ over Gaussians with

$$g_\rho(r) = P_\rho(r - r_\rho)\exp[-\eta_\rho(r - r_\rho)^2] \quad (26)$$

where P denotes a polynomial in $(x - x_\rho)$, $(y - y_\rho)$, $(z - z_\rho)$, has the form

$$(\rho\sigma|\tau\omega) = q_{\rho\sigma}q_{\tau\omega} \cdot F \quad (27)$$

$$q_{\rho\sigma} = \exp \left[-\frac{\eta_\rho \cdot \eta_\sigma}{\eta_\rho + \eta_\sigma} (r_\rho - r_\sigma)^2 \right] \quad (28)$$

Since F is slowly varying compared to the exponential this suggests to estimate the size of $(\rho\sigma|\tau\omega)$ by

$$|(\rho\sigma|\omega)| \approx q_{\rho\sigma}q_{\tau\omega} \quad (29)$$

The estimate (29) is independent of the polynomial P . For the general case of contracted basis sets we define on the shell level

$$\tilde{Q}_{NM} = \max_{\substack{\rho \in N \\ \sigma \in M}} q_{\rho\sigma} \quad (30)$$

where $\rho \in N$ runs over the primitives contracted in N . The estimate (29) then yields, independent of i

$$|(v\mu|\chi\lambda)| \approx |(v\mu|\chi\lambda)^i| \approx |(v\mu|\chi\lambda)^{ij}| \approx \tilde{Q}_{NM}\tilde{Q}_{KL} \quad (31)$$

The strategy outlined in the above charts clearly can be used with (31) instead of inequalities (8) and (9).

The relationship (29) provides only a rough estimate of the size of actual integrals or their derivatives, and detailed comparisons reveal the advantages of the rigorous bound (1) compared to (29).⁶ Rigorous bounds for two-electron integrals have been used only very recently in electronic structure calculations, e.g., in the program TURBOMOLE.³ Only for the special case of *s* type Gaussians has a rigorous bound been derived and used rather early,⁸ and this bound is actually a special case of (1).

RESULTS

Two systems were examined by comparing the rigorous bound with the simple estimate based on (31). All tests were performed on an IBM RISC SYSTEM/6000 workstation. The first system, the $(\text{H}_2\text{N})_2\text{PC}(\text{SiCH}_3)_3$ molecular ion was chosen for systematic tests both for the gradient and force modules of the TURBOMOLE package. The molecule was treated in C_{2v} symmetry using a 3-21G basis set which results in 146 basis functions. A more detailed description of the molecule is given in reference 9. The molecule was chosen because it has 15 atoms of medium size but consists of five different types of atoms. On the other hand, the molecule is not stretched—which would be the most fortunate case for prescreening—but relatively compact; such a shape will not give the best possible result.

For the second system, the molecule $[(\text{CF}_3)_2\text{PN}]_2\text{NVCl}_2$, a planar six-membered vanadin ring, we could only perform first-order gradient calculations. The calculations were performed in C_{2v} , too, and we used a DZP basis set for *N*, *C*, and *P*, and a SVP basis set for *V* leading to 336 basis functions. A detailed description of calculations performed on the molecule is given in reference 10. Test calculations were performed for various cut-off thresholds \mathcal{J} . All other parameters—MO vectors, molecular geometry, etc.—were kept constant in these calculations. We recorded the CPU time t_{CPU} for the evaluation and further processing of two-electron integral derivatives and the loss in accuracy. For this purpose we evaluated $\Delta x(\mathcal{J})$, for $x = g$ (gradient) and $x = h$ (Hessian), which results from neglecting contributions below the threshold \mathcal{J} , as indicated in the charts,

$$\Delta x(\mathcal{J}) = \|x(\mathcal{J}) - x_0\|, x = g \text{ or } h, \quad (32)$$

$x(\mathcal{J})$ denotes here the property computed in using the actual cut-off threshold, and x_0 the result obtained for the reference calculation with $\mathcal{J} = 10^{-20}$.

The results of our calculations are presented in Tables I and II. In Figures 1 to 3 we plot CPU times t_{CPU} vs. $-\log \Delta g$ and $-\log \Delta h$, which provides a direct measure of efficiency. The following conclusions emerge from these data.

Table I. Two-electron integral evaluation times and accuracy for $(\text{H}_2\text{N})_2\text{PC}(\text{SiCH}_3)_3$

Gradient \mathcal{J}^c	Method ^b	$\Delta x(\mathcal{J})^c$	$ g_{\text{max}} $	$t_{\text{CPU}}/\text{s}^d$
1E-20	B	0	0	3758
1E-10	B	0.3E-8	0.7E-8	2406
	A	0.4E-7	0.9E-7	2353
1E-9	B	0.3E-7	0.5E-7	2129
	A	0.2E-6	0.5E-6	2128
1E-8	B	0.2E-6	0.5E-6	1800
	A	0.1E-5	0.2E-5	1870
1E-7	B	0.3E-5	0.5E-5	1448
	A	0.3E-4	0.5E-4	1601
5E-7	B	0.2E-4	0.6E-4	1191
	A	0.4E-4	0.9E-4	1410
1E-6	B	0.4E-4	0.9E-4	1080
	A	0.7E-4	0.2E-3	1329
5E-6	B	0.3E-3	0.6E-3	820
	A	0.3E-3	0.1E-2	1132
Hessian				
1E-20	B	0	0	14998
1E-10	B	0.6E-7	0.1E-5	10534
	A	0.3E-7	0.6E-6	10578
1E-9	B	0.7E-7	0.1E-5	9451
	A	0.1E-6	0.2E-5	9776
1E-8	B	0.2E-5	0.4E-4	8227
	A	0.1E-4	0.3E-4	8908
1E-7	B	0.5E-5	0.1E-3	6897
	A	0.3E-5	0.4E-4	8029
5E-7	B	0.3E-4	0.5E-3	6177
	A	0.4E-4	0.5E-3	7597
1E-6	B	0.8E-4	0.1E-2	5509
	A	0.2E-4	0.3E-3	6689
5E-6	B	0.3E-3	0.4E-2	4485
	A	0.1E-3	0.2E-2	5938

^aComputational details are given in the text.

^bMethod A: prescreening by using estimate (31), method B: prescreening by using the rigorous bound (8), (9).

^cAccuracy defined by eq. (32).

^dTwo-electron integral evaluation time without time needed to get arrays *Q*, *R*, etc. (ca. 15 s).

^eIntegral neglecting threshold.

Table II. Two-electron evaluation time and accuracy for $[(\text{CF}_3)_2\text{PN}]_2\text{NVCl}_2^a$

\mathcal{J}	Method	$\Delta g(\mathcal{J})$	$ g_{\text{max}} $	t_{CPU}/s
Gradient				
1E-15	B	0	0	25014
1E-10	B	0.6E-8	0.1E-7	14010
1E-8	B	0.5E-6	0.9E-6	9595
	A	1.0E-5	0.1E-4	9473
1E-7	B	0.6E-5	0.1E-4	7452
	A	0.3E-4	0.7E-4	7700
5E-7	B	0.4E-4	1.0E-4	6018
	A	0.1E-3	0.3E-3	6475
1E-6	B	0.6E-4	0.2E-3	5420
	A	0.3E-3	0.6E-3	6060

^aComputational details are given in the text.

^bMethod A: prescreening by using estimate (31), method B: prescreening by using the rigorous bound (21).

^cAccuracy defined by eq. (32).

^dTwo-electron integral evaluation time without time needed to get arrays *Q*, *R*, etc. (ca. 35 s).

^eIntegral neglecting threshold.

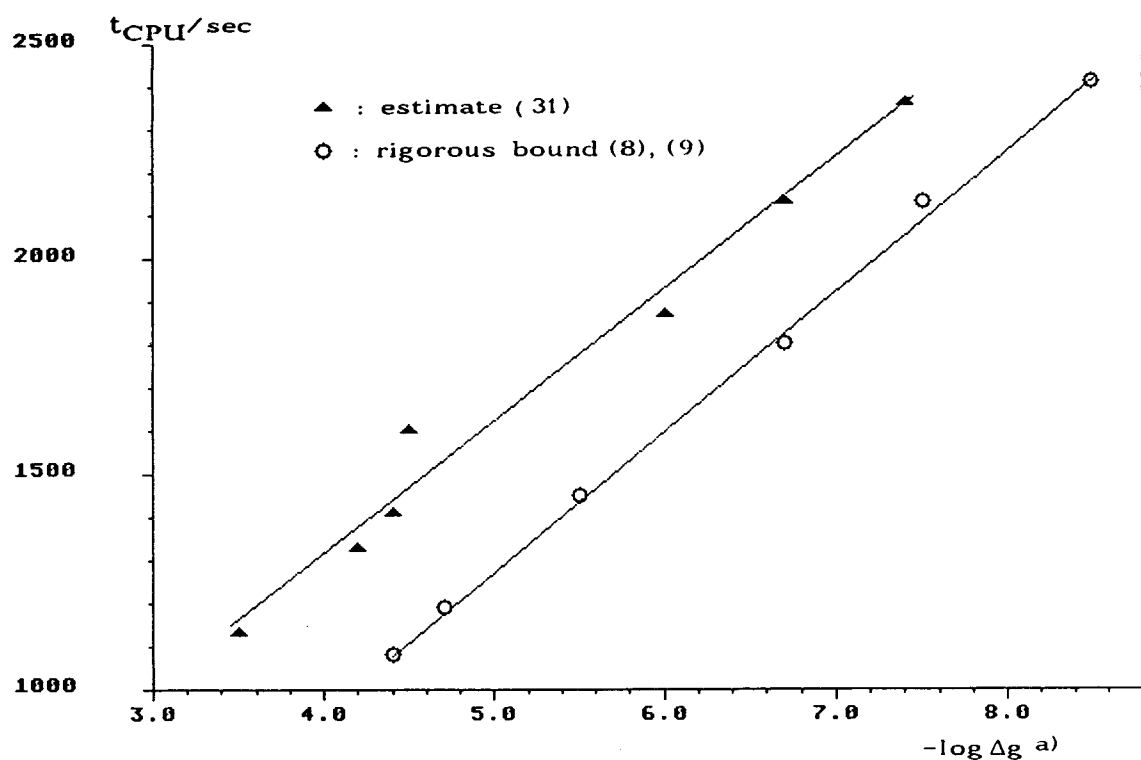


Figure 1. Two-electron integral evaluation time for first-order gradient calculations vs. accuracy for $(\text{H}_2\text{N})_2\text{PC}(\text{SiCH}_3)_3$. (Accuracy according to eq. (32). Without time needed to get arrays Q , R , etc. (ca. 15 s).)

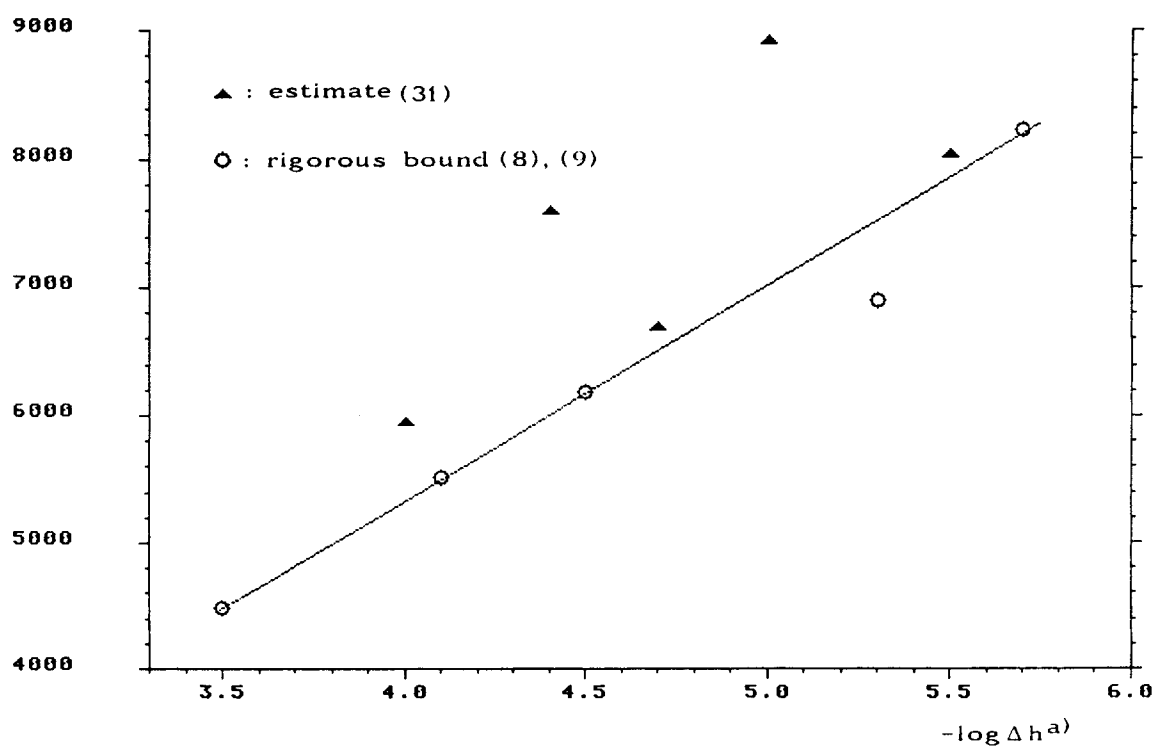


Figure 2. Two-electron integral evaluation time for Hessian calculation vs. accuracy for $(\text{H}_2\text{N})_2\text{PC}(\text{SiCH}_3)_3$. (Accuracy according to eq. (32). Without time needed to get arrays Q , R , etc. (ca. 300 s).)

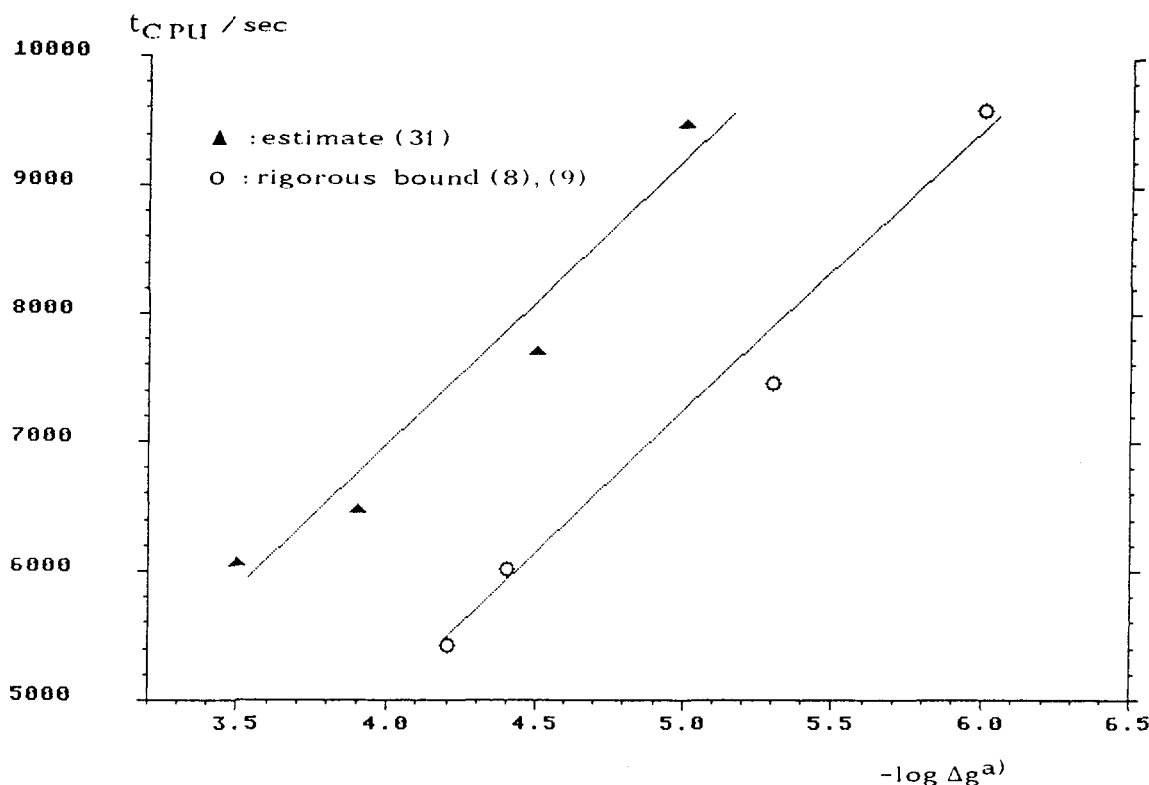


Figure 3. Two-electron integral evaluation time for the first-order gradient vs. accuracy for $[(CF_3)_2PN]_2NVCl_2$.¹⁰ (Accuracy according to eq. (32). Without time needed for to get arrays Q , R , etc. (ca. 35 s).

1. For the rigorous bound, eq. (3) and (8), (9), t_{CPU} varies linearly with $\log \Delta g$ and $\log \Delta h$ with relatively little scatter, at least in the region investigated. The amount of scatter is larger if prescreening is based on the estimate (31), especially for t_{CPU} vs. $-\log \Delta h$ (Fig. 2).
2. t_{CPU} vs. $-\log \Delta g$ for the rigorous bound is reduced by roughly a constant Δt (300 s in Figure 1 and 2000 s in Figure 3) as compared to using the estimate (31). This amounts to savings of 20 to 30% (or more) in t_{CPU} for a given accuracy Δg , depending on the actual Δg .
3. For fixed t_{CPU} the rigorous bound gains about an order of magnitude in accuracy in gradient calculations (Figs. 1 and 3).
4. The estimate (31) leads to a pronounced scatter in t_{CPU} vs. $-\log \Delta h$, (Fig. 2), whereas the rigorous bound still shows a smooth behavior. This requires using a tight cut-off threshold in connection with (31)—just to be on the safe side—and constitutes a definite advantage of the rigorous bound which is not easily quantified (20–50% in t_{CPU}).
5. The rigorous bound allows for a reliable estimate of the loss in accuracy. From the results presented in Tables I and II one obtains

$$\Delta x(g) \leq 100 \, g, \, x = g \text{ or } h \quad (33)$$

Our experience indicates this estimate to hold independently of circumstances for calculations with up to 500 basis functions; it also holds for

SCF-energy calculations. This opens the way to tailor the calculation to the desired accuracy.

6. We finally want to point out that the use of (1) is most efficient for energy calculations and less so for gradients and even less for the Hessian (as discussed in connection with chart two). The reason for this is obvious from a comparison of (1) with (11) and (12) which require additional use of triangular inequalities.

SUMMARY

We have derived rigorous bounds to derivatives of two-electron integrals required in gradient and Hessian calculations, e.g., eqs. (3) and (21). On the basis of these bounds it is extremely easy to skip the evaluation of near zero contributions to g and h , as demonstrated in the charts. Numerical tests show a definite advantage of using these rigorous bounds since the latter allow for a reliable assessment of the loss in accuracy resulting from neglect of small contributions to g or h . Usage of the present rigorous bounds also leads to advantages in accuracy and/or CPU time as compared to previously proposed estimates.

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