Geopotential

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2019-01-20

This document describes the computations that are performed by the method `GeneralSphericalHarmonicsAcceleration` of class `Geopotential` to determine the acceleration exerted by a non-spherical celestial on a point mass.

Notation

Let $\boldsymbol{r}$ be the vector going from the centre of the celestial to the point mass. Let $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}})$ be a (direct) base whose $\hat{\boldsymbol{z}}$ axis is along the axis of rotation of the celestial and whose $\hat{\boldsymbol{x}}$ axis points toward a reference point on the celestial. In this base $\boldsymbol{r}$ has coordinates (x, y, z) which can be expressed in terms of the latitude $\beta \in \left[\frac{\pi}{2}, \frac{\pi}{2}\right]$ and the longitude $\lambda \in [0, 2\pi]$:

$$\boldsymbol{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r\cos\beta\cos\lambda \\ r\cos\beta\sin\lambda \\ r\sin\beta \end{pmatrix}$$

where r is the norm of $\boldsymbol{r}$. Note that $\cos\beta > 0$, which will come handy when simplifying expressions like $\sqrt{1-\sin^2\beta}$.

Potential and acceleration

The gravitational potential due to the celestial has the form[PL10]:

$$U(\boldsymbol{r}) = -\frac{\mu}{r}\left(1 + \sum_{n=1}^{\infty}\sum_{m=0}^{n}\left(\frac{R}{r}\right)^n \mathrm{P}_{nm}(\sin\beta)(C_{nm}\cos m\lambda + S_{nm}\sin m\lambda)\right)$$

where P_{nm} is the associated Legendre function defined as[Rie+16, appendix]:

$$\mathrm{P}_{nm} = (1-t^2)^{\frac{m}{2}}\frac{\mathrm{d}^m\,\mathrm{P}_n(t)}{\mathrm{d}\,t^m}$$

The terms that are relevant for evaluating the acceleration exerted by the spherical harmonics on the point mass have the form:

$$V_{nm}(\boldsymbol{r}) = \frac{1}{r}\left(\frac{R}{r}\right)^n \mathrm{P}_{nm}(\sin\beta)(C_{nm}\cos m\lambda + S_{nm}\sin m\lambda)$$

and the acceleration itself is proportional to $\nabla V_{nm}(\boldsymbol{r})$.

$V_{nm}(\boldsymbol{r})$ can be written as the product of a radial term, a latitudinal term and a longitudinal term, dependent of r, β, and λ, respectively:

$$V_{nm}(\boldsymbol{r}) = \mathfrak{R}(r)\,\mathfrak{B}(\beta)\,\mathfrak{L}(\lambda)$$

where:

$$\begin{cases} \mathfrak{R}(r) & = \frac{1}{r}\left(\frac{R}{r}\right)^n \\ \mathfrak{B}(\beta) & = \mathrm{P}_{nm}(\sin\beta) \\ \mathfrak{L}(\lambda) & = C_{nm}\cos m\lambda + S_{nm}\sin m\lambda \end{cases}$$

The overall gradient can then be written as:

$$\nabla V_{nm}(\boldsymbol{r}) = \nabla\mathfrak{R}(r)\,\mathfrak{B}(\beta)\,\mathfrak{L}(\lambda) + \mathfrak{R}(r)\,\nabla\mathfrak{B}(\beta)\,\mathfrak{L}(\lambda) + \mathfrak{R}(r)\,\mathfrak{B}(\beta)\,\nabla\mathfrak{L}(\lambda)$$

Lemmata

To compute the acceleration, we first determine the gradient of various elements appearing in the potential. The following lemma determines the gradient of the $\mathfrak{R}$ term:

Lemma.

$$\nabla r^n = n r^{n-2} \boldsymbol{r}.$$

Proof. We have trivially:

$$\nabla r = \nabla\sqrt{x^2 + y^2 + z^2} = \frac{\boldsymbol{r}}{r}$$

from which we deduce:

$$\nabla r^n = n r^{n-1} \nabla r = n r^{n-2} \boldsymbol{r}$$

□

The following lemma is useful for computing the gradient of the $\mathfrak{B}$ term:

Lemma.

$$\nabla \sin\beta = \frac{\cos\beta}{r} \begin{pmatrix} -\sin\beta\cos\lambda \\ -\sin\beta\sin\lambda \\ \cos\beta \end{pmatrix}.$$

Proof. Noting that $\nabla z = \hat{\boldsymbol{z}}$ we have:

$$\nabla \sin\beta = \nabla\frac{z}{r} = \frac{r\hat{\boldsymbol{z}} - z r^{-1}\boldsymbol{r}}{r^2} = \frac{r^2\hat{\boldsymbol{z}} - z\boldsymbol{r}}{r^3}$$

which can be written, in coordinates:

$$\nabla \sin\beta = \frac{1}{r^3} \begin{pmatrix} -xz \\ -yz \\ x^2 + y^2 \end{pmatrix} = \frac{1}{r^3} \begin{pmatrix} -r^2 \sin\beta\cos\beta\cos\lambda \\ -r^2 \sin\beta\cos\beta\sin\lambda \\ r^2\cos^2\beta \end{pmatrix} = \frac{\cos\beta}{r} \begin{pmatrix} -\sin\beta\cos\lambda \\ -\sin\beta\sin\lambda \\ \cos\beta \end{pmatrix}$$

□

For the $\mathfrak{L}$ term, we will need to evaluate the quantities:

$$\begin{cases} \nabla \cos m\lambda & = -m \sin m\lambda \, \nabla\lambda \\ \nabla \sin m\lambda & = m \cos m\lambda \, \nabla\lambda \end{cases}$$

The following lemma helps with that computation:

Lemma.

$$\nabla\lambda = \frac{1}{r\cos\beta} \begin{pmatrix} -\sin\lambda \\ \cos\lambda \\ 0 \end{pmatrix}.$$

Proof. The angle λ is $\arctan\frac{y}{x}$ thus:

$$\nabla\lambda = \frac{1}{1 + \left(\frac{y}{x}\right)^2} \nabla\left(\frac{y}{x}\right) = \frac{1}{1 + \left(\frac{y}{x}\right)^2} \frac{x\hat{\boldsymbol{y}} - y\hat{\boldsymbol{x}}}{x^2} = \frac{x\hat{\boldsymbol{y}} - y\hat{\boldsymbol{x}}}{x^2 + y^2}$$

which can be written, in coordinates:

$$\nabla\lambda = \frac{1}{x^2 + y^2} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} = \frac{1}{r^2\cos^2\beta} \begin{pmatrix} -r\cos\beta\sin\lambda \\ r\cos\beta\cos\lambda \\ 0 \end{pmatrix} = \frac{1}{r\cos\beta} \begin{pmatrix} -\sin\lambda \\ \cos\lambda \\ 0 \end{pmatrix}$$

□

Finally, we will need the gradient of the associated Legendre polynomial, given by the following lemma:

Lemma.

$$\mathrm{P}'_{nm}(t) = (1-t^2)^{\frac{m}{2}} \frac{\mathrm{d}^{m+1}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m+1}} - mt(1-t^2)^{\frac{m-2}{2}} \frac{\mathrm{d}^{m}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m}}.$$

Proof. This follows trivially from the definition:

$$\mathrm{P}'_{nm}(t) = \frac{m}{2}(1-t^2)^{\frac{m}{2}-1}(-2t)\frac{\mathrm{d}^{m}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m}} + (1-t^2)^{\frac{m}{2}} \frac{\mathrm{d}^{m+1}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m+1}} \qquad \square$$

Gradients

We can now compute the gradient of the three terms that make up $V_{nm}(\boldsymbol{r})$. First, the radial term:

$$\nabla\mathfrak{R}(r) = R^n \nabla r^{-(n+1)} = -(n+1)R^n r^{-(n+3)}\boldsymbol{r} = -(n+1)\frac{\mathfrak{R}(r)}{r^2}\boldsymbol{r}$$

For the latitudinal term, the chain rule yields:

$$\nabla\mathfrak{B}(\beta) = \mathrm{P}_{nm}\big(\sin\beta\big)\,\nabla\sin\beta = \mathrm{P}'_{nm}\big(\sin\beta\big)\frac{\cos\beta}{r}\begin{pmatrix}-\sin\beta\cos\lambda\\ -\sin\beta\sin\lambda\\ \cos\beta\end{pmatrix}$$

Substituting $\sin\beta$ for the argument of P_{nm} and its derivative we obtain:

$$\begin{cases}\mathrm{P}_{nm}\big(\sin\beta\big) = \cos^m\beta\left.\dfrac{\mathrm{d}^{m}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m}}\right|_{t=\sin\beta}\\ \mathrm{P}'_{nm}\big(\sin\beta\big) = \cos^m\beta\left.\dfrac{\mathrm{d}^{m+1}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m+1}}\right|_{t=\sin\beta} - m\sin\beta\big(\cos\beta\big)^{m-2}\left.\dfrac{\mathrm{d}^{m}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m}}\right|_{t=\sin\beta}\end{cases}$$

and thus:

$$\begin{cases}\mathfrak{B}(\beta) = \cos^m\beta\left.\dfrac{\mathrm{d}^{m}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m}}\right|_{t=\sin\beta}\\ \nabla\mathfrak{B}(\beta) = \dfrac{1}{r}\left(\big(\cos\beta\big)^{m+1}\left.\dfrac{\mathrm{d}^{m+1}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m+1}}\right|_{t=\sin\beta} - m\sin\beta\big(\cos\beta\big)^{m-1}\left.\dfrac{\mathrm{d}^{m}\,\mathrm{P}_n(t)}{\mathrm{d}\,t^{m}}\right|_{t=\sin\beta}\right)\begin{pmatrix}-\sin\beta\cos\lambda\\ -\sin\beta\sin\lambda\\ \cos\beta\end{pmatrix}\end{cases}$$

For the longitudinal term we have:

$$\nabla\mathfrak{L}(\lambda) = (-mC_{nm}\sin m\lambda + mS_{nm}\cos m\lambda)\nabla\lambda = \frac{m}{r\cos\beta}(S_{nm}\cos m\lambda - C_{nm}\sin m\lambda)\begin{pmatrix}-\sin\lambda\\ \cos\lambda\\ 0\end{pmatrix}$$

Singularities

While the above formulæ are all we need to compute the gradient of the geopotential, they present a number of singularities that require some care for implementation purposes.

There is obviously a pole when $r = 0$. This one is not very interesting as we are never going to compute the acceleration at the centre of the celestial.

There are however removable singularities that arise when $\cos\beta$ appears at the denominator: any point on the axis of rotation of the celestial has $\cos\beta = 0$, but clearly the acceleration there is finite.

Consider $\nabla\mathfrak{B}(\beta)$. When $m = 0$ it includes a term in $(\cos\beta)^{-1}$. However, that term is multiplied by m, so it vanishes. Thus, for $m = 0$ we must use the special formula:

$$\nabla\mathfrak{B}(\beta)_{m=0} = \frac{\cos\beta}{r} \frac{\mathrm{d}\,\mathrm{P}_n(t)}{\mathrm{d}\,t}\bigg|_{t=\sin\beta} \begin{pmatrix} -\sin\beta\cos\lambda \\ -\sin\beta\sin\lambda \\ \cos\beta \end{pmatrix}$$

Similarly $\nabla\mathfrak{L}(\lambda)$ has $\cos\beta$ as its denominator. To eliminate this term we note that $\nabla\mathfrak{L}(\lambda)$ always occurs in a product involving $\mathfrak{B}(\beta)$. Let's write this product:

$$\mathfrak{B}(\beta)\nabla\mathfrak{L}(\lambda) = \frac{m(\cos\beta)^{m-1}}{r} \frac{\mathrm{d}^m\,\mathrm{P}_n(t)}{\mathrm{d}\,t^m}\bigg|_{t=\sin\beta} (S_{nm}\cos m\lambda - C_{nm}\sin m\lambda) \begin{pmatrix} -\sin\lambda \\ \cos\lambda \\ 0 \end{pmatrix}$$

When $m = 0$ this expression has a term in $(\cos\beta)^{-1}$ so we need to special-case it:

$$\mathfrak{B}(\beta)\nabla\mathfrak{L}(\lambda)_{m=0} = 0$$

Implementation considerations

A naïve implementation of the preceding formulæ yields poor performance because of the computation of trigonometric functions, powers and polynomials. It is advantageous to use simple geometric identities and recurrence formulæ to avoid these computations, at the expense of a small amount of storage. First, we note that:

$$x^2 + y^2 = r^2\cos^2\beta$$

and therefore we obtain the trigonometric functions for β:

$$\begin{cases} \cos\beta = \dfrac{\sqrt{x^2+y^2}}{r} \\ \sin\beta = \dfrac{z}{r} \end{cases}$$

and for λ:

$$\begin{cases} \cos\lambda = \dfrac{x}{\sqrt{x^2+y^2}} \\ \sin\lambda = \dfrac{y}{\sqrt{x^2+y^2}} \end{cases}$$

In the case where $\sqrt{x^2+y^2}$ is 0, any value will do for λ, so we can for instance pick $\cos\lambda = 1$ and $\sin\lambda = 0$.

The value of $\cos^m\beta$ may be computed by recurrence with a relative error growing like $O(m)$. If m is even, we have:

$$\begin{cases} h = \dfrac{m}{2} \\ \cos^m\beta = \left(\cos^h\beta\right)^2 \end{cases}$$

and if m is odd:

$$\begin{cases} h_1 = \left\lfloor \dfrac{m}{2} \right\rfloor \\ h_2 = m - h_1 \\ \cos^m\beta = \left(\cos^{h_1}\beta\right)\left(\cos^{h_2}\beta\right) \end{cases}$$

The value of $\cos m\lambda$ and $\sin m\lambda$ may similarly be computed using elementary trigonometric identities with an absolute error growing like $O(m^2)$. If m is even, we have:

$$\begin{cases} h = \dfrac{m}{2} \\ \cos m\lambda = (\cos h\lambda + \sin h\lambda)(\cos h\lambda - \sin h\lambda) \\ \sin m\lambda = 2\sin h\lambda\cos h\lambda \end{cases}$$

and if m is odd:

$$\begin{cases} h_1 = \left\lfloor \frac{m}{2} \right\rfloor \\ h_2 = m - h_1 \\ \sin m\lambda = \sin h_1\lambda \cos h_2\lambda + \cos h_1\lambda \sin h_2\lambda \\ \cos m\lambda = \cos h_1\lambda \cos h_2\lambda - \sin h_1\lambda \sin h_2\lambda \end{cases}$$

For the Legendre polynomials, we are looking for a recurrence relationship among terms of the form $\frac{\mathrm{d}^m \mathrm{P}_n(t)}{\mathrm{d}\,t^m}$. First note that these terms are 0 when $m > n$. We start with the recurrence defining the polynomials themselves:

$$n\,\mathrm{P}_n(t) = (2n-1)t\,\mathrm{P}_{n-1}(t) - (n-1)\,\mathrm{P}_{n-2}(t)$$

and we derive m times:

$$n\frac{\mathrm{d}^m \mathrm{P}_n(t)}{\mathrm{d}\,t^m} = (2n-1)\frac{\mathrm{d}^m (t\,\mathrm{P}_{n-1}(t))}{\mathrm{d}\,t^m} - (n-1)\frac{\mathrm{d}^m \mathrm{P}_{n-2}(t)}{\mathrm{d}\,t^m}$$

It's easy to verify, by recurrence, that:

$$\frac{\mathrm{d}^m (t\,\mathrm{P}_n(t))}{\mathrm{d}\,t^m} = t\frac{\mathrm{d}^m \mathrm{P}_n(t)}{\mathrm{d}\,t^m} + m\frac{\mathrm{d}^{m-1} \mathrm{P}_n(t)}{\mathrm{d}\,t^{m-1}}$$

so we end up with:

$$n\frac{\mathrm{d}^m \mathrm{P}_n(t)}{\mathrm{d}\,t^m} = (2n-1)\left(t\frac{\mathrm{d}^m \mathrm{P}_{n-1}(t)}{\mathrm{d}\,t^m} + m\frac{\mathrm{d}^{m-1} \mathrm{P}_{n-1}(t)}{\mathrm{d}\,t^{m-1}}\right) - (n-1)\frac{\mathrm{d}^m \mathrm{P}_{n-2}(t)}{\mathrm{d}\,t^m}$$

This recurrence starts with $\mathrm{P}_0(t) = 1, \mathrm{P}_1(t) = t$ and $\frac{\mathrm{d}\,\mathrm{P}_1(t)}{\mathrm{d}\,t} = 1$. It is similar to [Wes17, eqn. (12)] and makes it possible to efficiently evaluate $\left.\frac{\mathrm{d}^m \mathrm{P}_n(t)}{\mathrm{d}\,t^m}\right|_{t=\sin\beta}$ for increasing values of n and m.

Damping

In order to reduce the computational cost, we ignore high degree and order terms at long range. This is done by replacing $\mathfrak{R}(r)$ by $\sigma(r)\mathfrak{R}(r)$ in V_{nm}, where $\sigma(r) = 0$ for all $r > s_1$, and $\sigma(r) = 1$ for all $r < s_0$, so that the V_{nm} term vanishes at long range and is unaffected at short range.

In the force computations, this means that $\nabla\mathfrak{R}$ is replaced by

$$\nabla(\sigma\mathfrak{R}) = (\sigma'\mathfrak{R} + \sigma\mathfrak{R}')\frac{\boldsymbol{r}}{r}.$$

Sigmoid

Since we want the force to remain continuous, we need σ to be C^1; we achieve this by making σ the cubic Hermite interpolation on the non-constant interval $[s_0, s_1]$,

$$\sigma(r) = \begin{cases} 1 & \text{for } r \le s_0, \\ \frac{(r-s_1)^2(2r-3s_0+s_1)}{(s_1-s_0)^3} & \text{for } r \in [s_0, s_1], \\ 0 & \text{for } r \ge s_1. \end{cases}$$

The radial component of the acceleration resulting from V_{nm} is

$$\mu\nabla V_{nm} \cdot \frac{\boldsymbol{r}}{r} = \mu\frac{\mathrm{d}\,\sigma(r)\mathfrak{R}(r)}{\mathrm{d}\,r}\mathfrak{B}(\beta)\,\mathfrak{L}(\lambda).$$

We require that it and all its derivatives be monotone, i.e., that

$$\forall k \in \mathbb{N}^*, \frac{\mathrm{d}^{k+1}\,\sigma(r)\mathfrak{R}(r)}{\mathrm{d}\,r^{k+1}}\mathfrak{B}(\beta)\,\mathfrak{L}(\lambda)$$

have constant sign for $r \in [s_0, s_1]$.

Removing those factors that do not depend on r, this means that we must have

$$\forall r \in]s_0, s_1[, \frac{\mathrm{d}^{k+1}\, \sigma(r) r^{-(n+1)}}{\mathrm{d}\, r^{k+1}} \neq 0. \tag{1}$$

Proposition. *The smallest value of s_1 such that (1) holds for all $k \geq 0$ and $n \geq 2$ is $s_1 = 3s_0$.* □

Proof. We start by writing:

$$\sigma(r) = \sum_{m=0}^{3} a_m r^m$$

where:

$$\begin{cases} a_0 &= \dfrac{(s_1 - 3s_0){s_1}^2}{(s_1 - s_0)^3} \\ a_1 &= \dfrac{6 s_0 s_1}{(s_1 - s_0)^3} \\ a_2 &= \dfrac{-3(s_0 + s_1)}{(s_1 - s_0)^3} \\ a_3 &= \dfrac{2}{(s_1 - s_0)^3} \end{cases}$$

The function being derived in (1) is:

$$\sigma(r) r^{-(n+1)} = \sum_{m=0}^{3} a_m r^{-(n-m+1)}$$

The k-th derivative of r^{-n} for $n > 0$ is:

$$\frac{\mathrm{d}^k\, \sigma(r) r^{-n}}{\mathrm{d}\, r^k} = (-1)^k \frac{(n+k-1)!}{(n-1)!} r^{-(n+k)}$$

Whence:

$$\begin{aligned} \frac{\mathrm{d}^{k+1}\, \sigma(r) r^{-(n+1)}}{\mathrm{d}\, r^{k+1}} &= (-1)^{(k+1)} \sum_{m=0}^{3} a_m \frac{(n+k-m+1)!}{(n-m)!} r^{-(n+k-m+2)} \\ &= (-1)^{(k+1)} r^{-(n+k-m+2)} \frac{(n+k-2)!}{n!} \Big[a_0 (n+k+1)(n+k)(n+k-1) \\ &\qquad + a_1 (n+k)(n+k-1) n r \\ &\qquad + a_2 (n+k-1) n (n-1) r^2 \\ &\qquad + a_3 n (n-1)(n-2) r^3 \Big] \end{aligned}$$

Substituting the values of the (a_i), we see that the zeroes of $\frac{\mathrm{d}^{k+1}\, \sigma(r) r^{-(n+1)}}{\mathrm{d}\, r^{k+1}}$ are those of the polynomial:

$$\begin{aligned} d_{nk}(s_0, s_1; r) = {} & (s_1 - 3s_0){s_1}^2 (n+k+1)(n+k)(n+k-1) \\ & + 6 s_0 s_1 (n+k)(n+k-1) n r \\ & - 3(s_0 + s_1)(n+k-1) n (n-1) r^2 \\ & + 2n(n-1)(n-2) r^3 \end{aligned}$$

The following two lemmata establish properties of the roots of $d_{nk}(s_0, s_1; r)$:

Lemma (necessary condition). *If $s_1 < 3s_0$ then there exist k and n such that $d_{nk}(s_0, s_1; r)$ has a zero in $]s_0, s_1[$.* □

Lemma (sufficient condition). *If $s_1 = 3s_0$ then the positive roots of $d_{nk}(s_0, s_1; r)$ are greater than s_1.* □

These lemmata trivially constitute necessary and sufficient conditions, respectively, for the proposition. □

Proof (of necessary condition). In this proof we set $n = 2$, which causes the term in r^3 of $d_{nk}(s_0, s_1; r)$ to vanish:

$$d_{2,k}(s_0, s_1; r) = (s_1 - 3s_0)s_1^2(k+3)(k+2)(k+1) + 12s_0s_1(k+2)(k+1)r - 6(s_0+s_1)(k+1)r^2$$

The roots of $d_{2,k}(s_0, s_1; r)$ can be computed by solving:

$$(s_1 - 3s_0)s_1^2(k+3)(k+2) + 12s_0s_1(k+2)r - 6(s_0+s_1)r^2 = 0$$

The reduced discriminant of this equation is:

$$\begin{aligned}\Delta' &= 36s_0^2s_1^2(k+2)^2 + 6(s_0+s_1)(s_1-3s_0)s_1^2(k+2)(k+3)\\ &= 6s_1^2(k+2)(6s_0^2(k+2) + (s_1^2 - 2s_0s_1 - 3s_0^2)(k+3))\\ &= 6s_1^2(k+2)(k(s_1^2 - 2s_0s_1 + 3s_0^2) + 3(s_1-s_0)^2)\end{aligned}$$

and its solutions are:

$$r_\pm = s_1\frac{6s_0(k+2) \pm \sqrt{6(k+2)(k(s_1^2 - 2s_0s_1 + 3s_0^2) + 3(s_1-s_0)^2)}}{6(s_0+s_1)}$$

We are going to construct a value of k such that the smallest root r_- is in $]s_0, s_1[$. First, consider the inequality $r_- < s_1$. It can be rewritten:

$$\begin{aligned}& 6s_0(k+2) - 6(s_0+s_1) < \sqrt{6(k+2)(k(s_1^2 - 2s_0s_1 + 3s_0^2) + 3(s_1-s_0)^2)}\\ \Leftrightarrow\ & 6(ks_0 + (s_0 - s_1))^2 < (k+2)(k(s_1^2 - 2s_0s_1 + 3s_0^2) + 3(s_1-s_0)^2)\\ \Leftrightarrow\ & 6(k^2s_0^2 + 2ks_0(s_0-s_1) + (s_0-s_1)^2) <\\ & \qquad k^2(s_1^2 - 2s_0s_1 + 3s_0^2) + k(3(s_1-s_0)^2 + 2(s_1^2 - 2s_0s_1 + 3s_0^2)) + 6(s_0-s_1)^2\\ \Leftrightarrow\ & k^2(3s_0^2 + 2s_0s_1 - s_1^2) + k(12s_0(s_0-s_1) - 3(s_1-s_0) - 2(s_1^2 - 2s_0s_1 + 3s_0^2)) < 0\\ \Leftrightarrow\ & k(3s_0^2 + 2s_0s_1) + (3s_0^2 - 2s_0s_1 - 5s_1^2) < 0\\ \Leftrightarrow\ & k(3s_0 - s_1)(s_0+s_1) + (3s_0 - 5s_1)(s_0+s_1) < 0\\ \Leftrightarrow\ & k < \frac{5s_1 - 3s_0}{3s_0 - s_1}\end{aligned}$$

When s_1 is sufficiently close to $3s_0$, let's write $s_1 = 3(1-\epsilon)s_0$ with $\epsilon > 0$. The above inequality becomes:

$$k < \frac{15(1-\epsilon) - 3}{3\epsilon} = \frac{4}{\epsilon} + \mathcal{O}(1)$$

Similarly, the inequality $s_0 < r_-$ can be rewritten as follows:

$$\begin{aligned}& 6s_0s_1(k+2) - 6(s_0+s_1)s_0 > s_1\sqrt{6(k+2)(k(s_1^2 - 2s_0s_1 + 3s_0^2) + 3(s_1-s_0)^2)}\\ \Leftrightarrow\ & 6s_0^2(ks_1 + (s_1-s_0))^2 > s_1^2(k+2)(k(s_1^2 - 2s_0s_1 + 3s_0^2) + 3(s_1-s_0)^2)\\ \Leftrightarrow\ & 6s_0^2(k^2s_1^2 + 2ks_1(s_1-s_0) + (s_1-s_0)^2) >\\ & \qquad k^2s_1^2(s_1^2 - 2s_0s_1 + 3s_0^2) + ks_1^2(3(s_1-s_0)^2 + 2(s_1^2 - 2s_0s_1 + 3s_0^2)) + 6s_1^2(s_0-s_1)^2\\ \Leftrightarrow\ & k^2s_1^2(3s_0^2 + 2s_0s_1 - s_1^2) + ks_1(-5s_1^3 + 10s_0s_1^2 + 3s_0^2s_1 - 12s_0^3) + 6(s_0-s_1)^3(s_0+s_1) > 0\\ \Leftrightarrow\ & k^2s_1^2(3s_0 - s_1)(s_0+s_1) + ks_1(-5s_1^2 + 15s_0s_1 - 12s_0^2)(s_0+s_1) + 6(s_0-s_1)^3(s_0+s_1) > 0\\ \Leftrightarrow\ & k^2s_1^2(3s_0 - s_1) + ks_1(-5s_1^2 + 15s_0s_1 - 12s_0^2) + 6(s_0-s_1)^3 > 0\end{aligned}$$

Because the polynomial in k on the left-hand side of this inequality has a coefficient of k^2 which is positive when $s_1 < 3s_0$, the inequality is true if and only if k is greater that the largest root the polynomial. Using $s_1 = 3(1-\epsilon)s_0$ the roots can be found by solving:

$$9k^2(\epsilon + \mathcal{O}(\epsilon^2)) - 12k(1 + \mathcal{O}(\epsilon)) - 16(1 + \mathcal{O}(\epsilon)) = 0$$

Which yields the condition on k:

$$k > \frac{4}{3\epsilon} + \mathcal{O}(1)$$

When $k \to +\infty$ we have:

$$\Delta' = 6s_1^2k^2(s_1^2 - 2s_0s_1 + 3s_0^2) + \mathcal{O}(k)$$

and thus:

$$\sqrt{\Delta'} = s_1k\sqrt{6(s_1^2 - 2s_0s_1 + 3s_0^2)} + \mathcal{O}(1)$$

Hence, for the smallest root r_-:

$$r_- = k\frac{6s_0s_1 - s_1\sqrt{6(s_1^2 - 2s_0s_1 + 3s_0^2)}}{6(s_0 + s_1)} + \mathcal{O}(1)$$

This root tends to (positive) infinity if the numerator of the fraction is positive, that is if:

$$\begin{aligned} & 6s_0 > \sqrt{6(s_1^2 - 2s_0s_1 + 3s_0^2)} \\ \iff & 6s_0^2 > s_1^2 - 2s_0s_1 + 3s_0^2 \\ \iff & 3s_0^2 + 2s_0s_1 - s_1^2 > 0 \\ \iff & (3s_0 - s_1)(s_0 + s_1) > 0 \quad \text{which is true if and only if } s_1 < 3s_0. \end{aligned}$$

For $k = 0$, $d_{2,k}(s_0, s_1; r)$ has a root smaller than s_0. When $k \to +\infty$, its smallest root $r_- \to +\infty$. By continuity there exist values of k such that the smallest root is in $]s_0, s_1[$. ◻

Remark. The continuity argument in the above proof is not valid because $k \in \mathbb{N}$. ◊

Proof (of sufficient condition). With the choice $s_1 = 3s_0$ the constant term of $d_{nk}(s_0, s_1; r)$ vanishes and $r = 0$ is a trivial root. We are left with the equation:

$$6s_0s_1(n+k)(n+k-1) - 3(s_0 + s_1)(n+k-1)(n-1)r + 2(n-1)(n-2)r^2 = 0$$

or, substituting s_1:

$$9{s_0}^2(n+k)(n+k-1) - 6s_0(n+k-1)(n-1)r + (n-1)(n-2)r^2 = 0 \qquad (2)$$

The reduced discriminant of equation (2) is:

$$\begin{aligned} \Delta' &= 9{s_0}^2(n+k-1)^2(n-1)^2 - 9{s_0}^2(n+k)(n+k-1)(n-1)(n-2) \\ &= 9{s_0}^2(n+k-1)(n-1)(k+1) \end{aligned}$$

and its solutions are, when $n > 2$:

$$r_\pm = 3s_0\frac{(n+k-1)(n-1) \pm \sqrt{(n+k-1)(n-1)(k+1)}}{(n-1)(n-2)}$$

We want to prove that the smallest root, r_- verifies $r_- > 3s_0$. This inequality can be rewritten:

$$\begin{aligned} & (n+k-1)(n-1) - (n-1)(n-2) > \sqrt{(n+k-1)(n-1)(k+1)} \\ \iff & (n-1)(k+1) > \sqrt{(n+k-1)(n-1)(k+1)} \\ \iff & (n-1)(k+1) > n+k-1 \\ \iff & k(n-2) > 0 \quad \text{which is trivally true.} \end{aligned}$$

When $n = 2$ equation (2) further reduces to a first-degree equation with root $r = \frac{3}{2}s_0(k+2)$ which verifies $r \geq 3s_0$. Note however that the latter inequality is not strict, i.e., the value $3s_0$ may be reached if $k = 0$ and $n = 2$. ◻

Accordingly, we pick $s_1 = 3s_0$. The expression for σ on $[s_0, s_1]$ simplifies to

$$\sigma(r) = \frac{r(r-3s_0)^2}{4s_0^3} = \frac{r^3}{4s_0^3} - \frac{3r^2}{2s_0^2} + \frac{9r}{4s_0}.$$

Threshold

For a tolerance ε, we choose s_0 as the smallest distance such that the radial component of the force at s_0 does not exceed ε times the magnitude of the central force,

$$\max_{\lambda,\beta} \left| s_0^2 \mathfrak{R}'(s_0) \mathfrak{B}(\beta) \mathfrak{L}(\lambda) \right| = \varepsilon.$$

This maximum decomposes to

$$\max_{\lambda,\beta} \left| s_0^2 \mathfrak{R}'(s_0) \mathfrak{B}(\beta) \mathfrak{L}(\lambda) \right| = |s_0^2 \mathfrak{R}'(s_0)| \max_{\beta} \left| \mathfrak{B}(\beta) \right| \max_{\lambda} |\mathfrak{L}(\lambda)|.$$

The first factor is

$$|s_0^2 \mathfrak{R}'(s_0)| = s_0^2 \frac{(n+1)\mathfrak{R}(s_0)}{s_0} = (n+1)\frac{R^n}{s_0^n}.$$

We have

$$\begin{aligned}
\max_{\lambda} |\mathfrak{L}(\lambda)| &= \max_{\lambda} |C_{nm} \cos m\lambda + S_{nm} \sin m\lambda| \\
&= \max_{\lambda} |\mathrm{Re}((C_{nm} + \mathrm{i} S_{nm}) \mathrm{e}^{-\mathrm{i}m\lambda})| \\
&= |C_{nm} + \mathrm{i} S_{nm}| = \sqrt{C_{nm}^2 + S_{nm}^2},
\end{aligned}$$

and we numerically compute and tabulate

$$\max_{\beta} \left| \mathfrak{B}(\beta) \right| = \max_{\beta} \left| \mathrm{P}_{nm}(\sin\beta) \right|.$$

Thus we can compute the desired s_0 as

$$s_0 = R \left(\frac{\max_\beta \left| \mathrm{P}_{nm}(\sin\beta) \right| (n+1) \sqrt{C_{nm}^2 + S_{nm}^2}}{\varepsilon} \right)^{\frac{1}{n}}.$$

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