Sensitivity Approximation and Verification

Solution to Harmonic Oscillator

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This part of the documentation justifies the expressions used in `verify.R` where we check the results of the sensitivity approximation method against the expected analytical result. The solution to the initial value problem of the Harmonic Oscillator is of course well known. The important part is its parameter-sensitivity (parameter derivative). We treat the damping parameter c as a system input and the coefficiant k of the main *restoring force* as the *interesting* parameter for sensitivity calculations. This choice is arbitrary.

1 Model Definition

We will use a dampened harmonic oscillator model with unit mass:

$$\ddot{y} = -ky - c\dot{y}\,, \tag{1}$$

to compare numerical k-sensitivity approximation methods to the analytical solution sensitivity. This model is well suited for the purpose of illustration as the sensitivity is a scalar function.

To use ordinary differential equation solvers, we reformulate the model as a system of equatuions, with order one:

$$\begin{aligned}
\dot{v} &= -ky - cv\,, & v(0) &= v_0 \qquad (2)\\
\dot{y} &= v\,, & y(0) &= y_0 \qquad (3)\\
& & & \qquad (4)
\end{aligned}$$

This system has a known analytical solution:

$$
\begin{aligned}
\omega &= \sqrt{k}\,, \\
r &= \frac{c}{2\omega}\,, \\
\Rightarrow r\omega &= \frac{c}{2}\,, \\
y(t;k) &= a\exp(-r\omega t)\cos(\sqrt{1-r^2}\omega t + \phi)\,, \\
\Rightarrow v(t;k) &= -a\exp(-r\omega t)(r\omega)\cos(\sqrt{1-r^2}\omega t + \phi) \\
&\quad - a\exp(-r\omega t)\sin(\sqrt{1-r^2}\omega t + \phi)\sqrt{1-r^2}\omega\,, \\
&= -y(t;k)\left(r\omega + \tan(\sqrt{1-r^2}\omega t + \phi)\sqrt{1-r^2}\omega\right)\,,
\end{aligned}
\tag{5}
$$

where a and ϕ are to be determined from the initial conditions v_0 and y_0:

$$
\begin{aligned}
&y(0;k) = a\cos(\phi) = y_0\,, \\
&v(0;k) = -y_0 r\omega - y_0\tan(\phi)\sqrt{1-r^2}\omega = v_0\,,
\end{aligned}
\tag{6}
$$

In Section 2 we show that (5) solves the ordinary differential equation (1).

All four constants a, ω, ϕ, and r are functions of (k, c), so we could instead write: $a(k, c)$, $r(k, c)$, etc.. But, to ease notation and avoid too many parentheses, we will instead note the dependence on k via subscripts. Since we are interested in the sensitivity of y only with repsect to k we will drop the dependence on c in notation.

1.1 Phase and Amplitude

We solve the initial value equations (6) for ϕ:

$$
\frac{v_0 + y_0 r_k \omega_k}{y_0\sqrt{1-r_k^2}\omega_k} = -\tan(\phi_k)\,, \tag{7}
$$

$$
\arctan\left(-\frac{2v_0 + y_0 c}{2y_0\sqrt{1-r_k^2}\omega_k}\right) = \phi_k\,. \tag{8}
$$

Here, we note that this solution for ϕ is also a function of k and append this note as a subscript. This result makes a immediately available as

$$
a_k = \frac{y_0}{\cos(\phi_k)}\,, \tag{9}
$$

where we make the dependence on k noted once again. We disregard the dependence on

1.2 Sensitivity

Because we are calculating the derivative with respect to k it is useful to rewrite the solution and make it explicit when a term does depend on k, and show where k cancels:

$$\begin{aligned} \Gamma_k &:= \sqrt{1-r_k^2}\,, \\ \Gamma_k\omega_k &= \sqrt{1-\left(\frac{c}{2\sqrt{k}}\right)^2}\sqrt{k} = \sqrt{k-\frac{c^2k}{4k}} = \sqrt{k-\frac{c^2}{4}}\,, \\ \Rightarrow y(t;k) &= a\exp\left(-\frac{c}{2}t\right)\cos\left(t\sqrt{k-\frac{c^2}{4}}+\phi_k\right)\,, \end{aligned} \tag{10}$$

The sensitivity of the solution $y(t;k)$ with respect to the parameter k can be obtained by straight forward differentiation, albeit with many terms. We collect a list of derivatives:

$$a_k = \frac{y_0}{\cos(\phi_k)} \qquad \frac{da_k}{dk} = \frac{y_0\tan(\phi_k)}{\cos(\phi_k)}\frac{d\phi_k}{dk} = a_k\tan(\phi_k)\frac{d\phi_k}{dk}\,, \tag{11}$$

$$\omega_k = \sqrt{k} \qquad \frac{d\omega_k}{dk} = \frac{1}{2\sqrt{k}}\,, \tag{12}$$

$$r_k = \frac{c}{2\omega_k} \qquad \frac{dr_k}{dk} = -\frac{c}{2\omega_k^2}\frac{d\omega_k}{dk} = -\frac{c}{2k}\frac{1}{2\sqrt{k}} = -\frac{r_k}{2k}\,, \tag{13}$$

$$r_k\omega_k = \frac{c}{2} \qquad \frac{d(r_k\omega_k)}{dk} = 0\,, \tag{14}$$

$$\Gamma_k = \sqrt{1-r_k^2} \qquad \frac{d\Gamma_k}{dk} = \frac{2r_k}{2\sqrt{1-r_k^2}}\frac{dr_k}{dk} = -\frac{r_k}{k}\frac{r_k}{2\Gamma_k}\,, \tag{15}$$

$$\Gamma_k\omega_k = \sqrt{k-\frac{c^2}{4}} \qquad \frac{d(\Gamma_k\omega_k)}{dk} = \frac{1}{2\sqrt{k-\frac{c^2}{4}}} = \frac{1}{2\Gamma_k\omega_k}\,, \tag{16}$$

First we take the derivative of ϕ from (7):

$$-\frac{d}{dk}\left(\frac{2v_0+y_0c}{2y_0\Gamma_k\omega_k}\right) = \frac{2}{cos(2\phi+1)}\frac{d\phi}{dk}\,, \tag{17}$$

$$-\left(-\frac{2v_0+y_0c}{4y_0(\Gamma_k\omega_k)^3}\right) = \frac{2}{cos(2\phi+1)}\frac{d\phi_k}{dk}\,, \tag{18}$$

We solve for the derivative of ϕ:

$$\frac{d\phi_k}{dk} = \cos(2\phi_k+1)\frac{2v_0+y_0c}{8y_0(\Gamma_k\omega_k)^3}\,, \tag{19}$$

```
w <- function(k) sqrt(k)
r <- function(k) c/(2*w(k))                               # damping ratio
srr1 <- function(k) sqrt(1-r(k)^2)                        # convenience
## srr1*w
srr1w <- function(k) sqrt(k-0.25*c^2)
## phase and amplitude
f <- function(k) atan(-(2*v0+y0*c)/(2*y0*srr1w(k)))
a <- function(k) y0/cos(f(k))
## derivatives
dwdk <- function(k) 1/(2*w(k))
dfdk <- function(k) cos(2*f(k) + 1)*(2*v0 + y0*c)/(8*y0*srr1w(k)^3)
dadk <- function(k) y0 * (tan(f(k))/cos(f(k))) * dfdk(k)
## y and S = dy/dk
y <- function(x,k) a(k)*exp(-0.5*c*x)*cos(srr1w(k)*x + f(k))
S <- function(x,k) {
  y(x,k)*(  tan(f(k))*dfdk(k)
          - tan(srr1w(k)*x+f(k))*(0.5*x/srr1w(k) + dfdk(k)))
}
```

Listing 1: Calculation of the sensitivity in R. The variables have slightly different names: `srr1(k)` is Γ_k and `srr1w(k)` is $\Gamma_k\omega_k$. The independent variable t is `x` in the code.

Using these results, we assemble the full sensitivity:

$$\begin{aligned}
\frac{dy(t;k)}{dk} &= \frac{d}{dk}\left(a_k \exp\left(-\frac{c}{2}t\right)\cos(\Gamma_k\omega_k t + \phi_k)\right), \\
&= \exp\left(-\frac{c}{2}t\right)\frac{d}{dk}\left(a_k\cos(\Gamma_k\omega_k t+\phi_k)\right), \\
&= \exp\left(-\frac{c}{2}t\right)\left(\frac{da_k}{dk}\cos(\Gamma_k\omega_k t+\phi_k) - a_k\sin(\Gamma_k\omega_k t+\phi_k)\left(\frac{t}{2\Gamma_k\omega_k}+\frac{d\phi_k}{dk}\right)\right), \\
&= \exp\left(-\frac{c}{2}t\right)\left(a_k\tan(\phi_k)\frac{d\phi_k}{dk}\cos(\Gamma_k\omega_k t+\phi_k) - a_k\sin(\Gamma_k\omega_k t+\phi_k)\left(\frac{t}{2\Gamma_k\omega_k}+\frac{d\phi_k}{dk}\right)\right), \\
&= y(t;k)\left(\tan(\phi_k)\frac{d\phi_k}{dk} - \tan(\Gamma_k\omega_k t+\phi_k)\left(\frac{t}{2\Gamma_k\omega_k}+\frac{d\phi_k}{dk}\right)\right),
\end{aligned} \tag{20}$$

The last line is suitable for direct evaluation, given the parameters (k, c). In R we calculate this using the function defined in Listing 1.

2 Proof for the Solution

We insert the proposed solution (5) into (1). First we perform al needed derivatives:

$$\begin{aligned}
y(t;k) &= a\exp(-r\omega t)\cos(\sqrt{1-r^2}\omega t+\phi), \\
\dot{y}(t;k) &= -y(t;k)r\omega - a\exp(-r\omega t)\sin(\sqrt{1-r^2}\omega t+\phi)\sqrt{1-r^2}\omega,
\end{aligned} \tag{21}$$

The second derivative of y:

$$\begin{aligned}\ddot{y}(t;k) = -\dot{y}(t;k)r\omega \\ - \Big(a \exp(-r\omega t)(-r\omega) \sin(\sqrt{1-r^2}\omega t + \phi)\sqrt{1-r^2}\omega \\ + a \exp(-r\omega t) \cos(\sqrt{1-r^2}\omega t + \phi)\left(\sqrt{1-r^2}\omega\right)^2\Big) ,\end{aligned} \tag{22}$$

which simplifies to:

$$\begin{aligned}\ddot{y}(t;k) &= -\dot{y}(t;k)r\omega - \left(\underbrace{-a \exp(-r\omega t) \sin(\sqrt{1-r^2}\omega t + \phi)\sqrt{1-r^2}\omega}_{\dot{y}+yr\omega} r\omega + y(t;k)\left(\sqrt{1-r^2}\omega\right)^2\right) ,\\ &= -\dot{y}(t;k)r\omega - \left(\dot{y}(t;k)r\omega + y(t;k)(r\omega)^2 + y(t;k)\left(\sqrt{1-r^2}\omega\right)^2\right) ,\\ &= -2\dot{y}(t;k)r\omega - \left(y(t;k)(r\omega)^2 + y(t;k)(1-r^2)\omega^2\right) ,\\ &= -2\dot{y}(t;k)r\omega - \left(y(t;k)\omega^2\right) ,\\ &= -2\dot{y}(t;k)\frac{c}{2} - y(t;k)k = -ky(t;k) - c\dot{y}(t;k) ,\end{aligned} \tag{23}$$

which reconstructs the original ODE in (1).