NONLINEAR MECHANICAL SYSTEMS

CANONICAL TRANSFORMATIONS AND NUMERICAL INTEGRATION

Jacobi Canonical Transformations

Jacobi canonical transformations are one particularly important subclass of canonical transformations. Any change of variables which results in a Hamiltonian which depends on only one of the conjugate variable sets is a Jacobi canonical transformation. As we have seen above, momentum and displacement can be interchanged, so it makes no difference whether the transformed Hamiltonian depends only on displacements or only on momenta, so we will follow Jacobi's convention and assume dependence on momentum alone. In the new variables

\[ H(p^*, q^*) = K(p^*) \]

\[ \frac{\partial K(p^*)}{\partial q^*} = 0 \]

Thus

\[ \frac{dp^*}{dt} = e^* \]

\[ \frac{dq^*}{dt} = \frac{\partial K(p^*)}{\partial p^*} - f^* \]

In effect, a Jacobi canonical transformation defines a set of variables in which the simple relation between effort and the rate of change of momentum is recovered.

EXAMPLE: SIMPLE HARMONIC OSCILLATOR

The Hamiltonian must be a quantity which is invariant under changes of variables. An obvious choice is the total system energy, but remember that the Hamiltonian does not have to be identified with energy; other invariants may be used.

\[ H(p, q) = \frac{1}{2}(p^2/I + q^2/C) \]

Hamilton's equations

\[ \frac{dq}{dt} = \frac{\partial H}{\partial p} = p/I \]

\[ \frac{dp}{dt} = -\frac{\partial H}{\partial q} = q/C \]
Change variables from the old conjugate pair $q, p$ to the new conjugate pair $P, Q$. Define $Z_0 = \sqrt{IC}$ and the generating function

$$S(q, Q) = Z_0 \left( \frac{q^2}{2} \right) \cot Q$$

The transformation equations are

$$p = \frac{\partial S}{\partial q} = Z_0 q \cot Q$$
$$P = -\frac{\partial S}{\partial Q} = Z_0 \left( \frac{q^2}{2} \right) / \sin^2 Q$$

Rewriting these equations to express the old variables in terms of the new

$$p = \sqrt{2P} \cos Q \sqrt{Z_0}$$
$$q = \sqrt{2P} \sin Q \left( \frac{1}{\sqrt{Z_0}} \right)$$

Defining $\omega_0 = \sqrt{1/IC}$ the new Hamiltonian is:

$$H(P, Q) = \omega_0 P = K(P)$$

In the new coordinates, the Hamiltonian state equations are particularly simple.

$$\frac{dQ}{dt} = \frac{\partial K}{\partial P} = \omega_0$$
$$\frac{dP}{dt} = -\frac{\partial K}{\partial Q} = 0$$

Their solution is

$$Q = \omega_0 t + \text{constant}$$
$$P = \text{constant}$$

We can give the transformed variables a physical interpretation: $P$ is proportional to the total energy in the system, and its square root is proportional to the amplitude of the oscillations; $Q$ is the phase angle of the oscillations. In essence the change of variables has integrated the equations, and this change of variables is also known as Jacobi's method of integration. The product of $P$ and $Q$ has the units of action (energy by time) and this canonical transformation has been called the simple harmonic actional transformation.

A Jacobi canonical transformation is an effective way to simplify the equations of a nonlinear dynamic system. A general method exists for
finding such transformations, but it is not trivial to apply as it requires the 
solution of a partial differential equation. However, Brouwer's extension of 
the Hamiltonian equations is sufficiently general to permit a practical 
alternative. A useful technique is to separate the Hamiltonian into a part 
for which a Jacobi canonical transform is known, and a part for which no 
Jacobi canonical transform is known.

\[ H(p,q) = H_j(p,q) + H_n(p,q) \]

Apply a Jacobi canonical transformation

\[ H^*(P,Q) = H^*_j(P) + H^*_n(P,Q) \]

Now we may represent the second term as a set of canonical forces

\[
e^*(P,Q) = -\frac{\partial H^*_n}{\partial Q}
\]

\[
f^*(P,Q) = -\frac{\partial H^*_n}{\partial P}
\]

The transformed equations become

\[
dP/dt = e^*(P,Q) 
\]

\[
dQ/dt = \frac{\partial H^*_j}{\partial P} - f^*(P,Q)
\]

An advantage of this change of variables is that, in effect, it integrates the 
oscillatory part of the solution.

**EXAMPLE: SIMPLE PENDULUM**

For large amplitude motions, the simple pendulum is a nonlinear oscillator. 
Using the angle with respect to the vertical as a coordinate, the 
Hamiltonian has the following form

\[
H(\eta, \theta) = \frac{\eta^2}{2} + 1 - \cos \theta
\]

(Length and time scales can always be chosen to simplify a problem in this 
way)

Expanding the cosine as a power series, we see that the Hamiltonian is a 
quadratic in momentum and displacement with extra terms in 
displacement of fourth and higher power.

\[
H(\eta, \theta) = \frac{\eta^2}{2} + \frac{\theta^2}{2} - \frac{\theta^4}{4!} + \frac{\theta^6}{6!} - \ldots
\]

From this we can see that until the fourth power of the angle in radians 
becomes significant, the simple pendulum may be treated as linear system.
For the quadratic terms, we know a Jacobi canonical transformation: the simple harmonic actional. The Hamiltonian can be decomposed into two terms as follows
\[ H(\eta, \theta) = \frac{\eta^2}{2} + \frac{\theta^2}{2} + (1 - \cos \theta - \frac{\theta^2}{2}) \]
\[ H(\eta, \theta) = K(\eta, \theta) + N(\eta, \theta) \]
Now apply the simple harmonic actional
\[ \theta = \sqrt{2P} \sin Q \]
\[ \eta = \sqrt{2P} \cos Q \]
The Hamiltonian becomes
\[ H^*(P,Q) = K^*(P) + N^*(P,Q) \]
In the original variables, the system equations are
\[ \frac{d\eta}{dt} = -\frac{\partial H}{\partial \theta} \]
\[ \frac{d\theta}{dt} = \frac{\partial H}{\partial \eta} \]
In the new variables, the system equations become
\[ \frac{dP}{dt} = -\frac{\partial N^*}{\partial Q} \]
\[ \frac{dQ}{dt} = 1 + \frac{\partial N^*}{\partial P} \]
To evaluate these terms, we take advantage of the fact that a canonical transformation preserves the value of the Hamiltonian and use the chain rule on the original \( N \) which in this case depends only on \( \theta \).
\[ \frac{\partial N^*}{\partial Q} = \left( \frac{\partial N}{\partial \theta} \right) \left( \frac{\partial \theta}{\partial Q} \right) \]
\[ \frac{\partial N^*}{\partial P} = \left( \frac{\partial N}{\partial \theta} \right) \left( \frac{\partial \theta}{\partial P} \right) \]
\[ \frac{\partial N}{\partial \theta} = \sin \theta - \theta \]
\[ \frac{\partial \theta}{\partial Q} = \sqrt{2P} \cos Q \]
\[ \frac{\partial \theta}{\partial P} = \sin Q \left( \frac{1}{\sqrt{2P}} \right) \]
Thus the transformed equations become
\[ \frac{dP}{dt} = [\sqrt{2P} \sin Q - \sin(\sqrt{2P} \sin Q)] [\sqrt{2P} \cos Q] \]
\[ \frac{dQ}{dt} = 1 + [\sin(\sqrt{2P} \sin Q) - \sqrt{2P} \sin Q][\sin Q \left( \frac{1}{\sqrt{2P}} \right)] \]
These nonlinear state equations don't look particularly simple. However, when we simulate the system we will probably be interested in the behavior in the original coordinates, so we will need two output equations, the transformation equations relating old variables to new. But we can use these output equations to simplify the state equations by expressing the rates of change as a function of both old and new variables. Collecting equations:

\[
\frac{dP}{dt} = (\theta - \sin \theta) \eta
\]

\[
\frac{dQ}{dt} = 1 + (\sin \theta - \theta) \theta / 2P
\]

\[
\theta = \sqrt{2P} \sin Q
\]

\[
\eta = \sqrt{2P} \cos Q
\]

Now, hold on a minute: in the old variables, the system equations are quite simple,

\[
\frac{d\eta}{dt} = -\sin \theta
\]

\[
\frac{d\theta}{dt} = \eta
\]

far simpler than the transformed equations, so what have we gained? In fact, quite a lot. In the new variables, the solution is far more stable numerically.
These equations were both integrated using a simple Euler integration algorithm (starting time 0 seconds, final time 50 seconds, time step 0.1 seconds. Starting the pendulum from equilibrium at an angle of 0.1 radians (≈6°) the original form is unstable. Total system energy, which should be constant, grows exponentially. In contrast, using the transformed equations, the simulation is stable. Total system energy is not constant, but its deviations are tiny, 5.6x10^-7.
Of course, there are more sophisticated algorithms available. If we perform the same integration using a third-order fixed-step Runge-Kutta algorithm, the result is as follows.

This looks fine until you examine the computed total system energy, which declines steadily by $2.1 \times 10^{-5}$ over 50 seconds. Using the same algorithm with the transformed equations yields
In this case, the total energy also decreases, but by $2.3 \times 10^{-10}$ — a hundred thousand time less.

Starting the pendulum from equilibrium at 1 radian ($\approx 57^\circ$) and using the same integration algorithm and integration parameters produces the following results.

Again, the transformed equations produce a smaller decline in energy, though the difference is less pronounced — $8.8 \times 10^{-4}$ vs. $1.5 \times 10^{-4}$. 
Things get a little more interesting when we start the pendulum from equilibrium at 5° off vertically upright (3.05 radians). Using the same integration algorithm and integration parameters produces the following results.

Now the original formulation is unstable, producing an energy increase of 1.3x10^-3 in 50 seconds. The transformed equations yield a decline of energy of 3.1x10^-3.
By the standards of the ‘90’s, fixed-step integration algorithms are considered crude. Newer algorithms adaptively change the integration step size to preserve accuracy. Starting from the same initial conditions but using MATLAB’s default integration algorithm (ode23, a third-order Runge-Kutta algorithm with error tolerance of $1.0 \times 10^{-3}$) produces the following results.
Now the steady increase in computed total energy in the original formulation results in a major departure of the computed angle from what it should be — the simulation claims that after one oscillation the pendulum will spin continuously in one direction. The transformed equations do not exhibit this behavior, though the computed energy declines substantially (9.3x10^-2 in 50 seconds).

**POINTS:**

- Never believe anything you get from a computer. Find some way of cross checking the results. One effective method is to compute a known invariant, in this case energy.

- The equations in the original variables may look simpler, but that is deceptive. In fact the transformed equations have been partially integrated by the transformation and so present a less demanding task to the integration algorithm.

- A little analysis up front can have a dramatic effect on the accuracy of numerical computations.

Bear in mind that the simple harmonic actional is only one member of the class of Jacobi canonical transformations. It is particularly useful as it provides a way to simplify the equations of an oscillatory system. If the Hamiltonian of the oscillator is quadratic, the simple harmonic actional completely integrates the equations for an undamped system. With damping, the rate of change of system energy is directly proportional to the canonical effort in the transformed variables.