Lagrangian Formulation vs. Hessian Analysis: Normal modes

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- **Lagrangian Formulation:** Focuses on **dynamics** (how systems move over time).
- **Hessian Matrix:** Focuses on system **properties** (stability and frequencies).
- Both are essential, complementary tools for comprehensive modeling.

Introduction & Core Concepts:contd..

The characterization of mechanical systems exhibiting oscillatory behavior, such as spring-mass models, necessitates rigorous mathematical frameworks. This document compares two fundamental analytical approaches: the **Lagrangian formulation** and the **Hessian matrix** analysis. The Lagrangian approach, rooted in variational calculus and scalar energy potentials, provides a systematic derivation of the governing equations of motion. Conversely, the Hessian matrix, a tool from multivariable calculus, serves a critical role in the stability analysis and identification of natural frequencies for these systems. Understanding the distinct roles and interconnectedness of these methods is crucial for comprehensive dynamic system modeling and analysis.

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Core Principle: Hamilton's Principle using $L = T - V$ (Kinetic - Potential Energy).

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4. **Result:** The equations of motion $[M]\ddot{\mathbf{x}} + [K]\mathbf{x} = \mathbf{0}$.

Application: Normal Mode Analysis in Computational Physics

- Normal Mode Analysis (NMA) is a direct application of the Hessian's Spectral Decomposition used extensively in molecular dynamics and materials science to study how systems vibrate. Just like a guitar string has certain allowed vibration patterns ("notes"), an n-mass spring system has certain allowed oscillation patterns called normal modes.

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  Consider a system of N atoms (or masses) connected by springs (chemical bonds). The potential energy V of the system is a function of the displacement vectors of all atoms, $\mathbf{q} = (q_1, q_2, \ldots, q_{3N})$.

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- We approximate the potential energy function $V(\mathbf{q})$ around a minimum energy geometry ($\mathbf{q}_0 = \mathbf{0}$) using the Taylor Series (construction of Hessian: will be described soon).

The Hessian Matrix: Stability Analysis

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- The Hessian matrix **is** the stiffness matrix $[K]$ at equilibrium.
- Used for eigenvalue analysis to find natural frequencies ω.

What is the Hessian?

The Hessian matrix captures second-order derivatives:

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

It is symmetric under mild smoothness assumptions and encodes curvature information for multivariate functions.

Gradient vs. Hessian

- **Gradient:** direction of steepest ascent, first derivative.
- **Hessian:** curvature (how gradient changes), second derivative.
- Symmetry: $H_{ij} = H_{ji}$ when second derivatives are continuous.

Gradient vs. Hessian

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- First Derivative: The Gradient (∇f). The gradient vector tells us the direction and rate of steepest ascent at a given point. It is crucial for finding stationary points where $\nabla f = \mathbf{0}$.
- Second Derivative: The Hessian ($\mathbf{H}$) The Hessian tells us about the curvature of the function at a stationary point. This curvature determines whether the point is a minimum, a maximum, or a saddle point.
  The Hessian is constructed as the matrix of all second-order partial derivatives:

2D Example: Function

Consider

$$f(x, y) = 2x^3 - 6xy + 3y^2.$$

Gradient:

$$\nabla f = \begin{pmatrix} 6x^2 - 6y \\ -6x + 6y \end{pmatrix}$$

Stationary points: $(0, 0)$ and $(1, 1)$.

2D Example: Hessian & Classification

Hessian:

$$H(x,y) = \begin{pmatrix} 12x & -6 \\ -6 & 6 \end{pmatrix}$$

At $(0,0)$: eigenvalues mixed $\Rightarrow$ saddle.
At $(1,1)$: eigenvalues positive $\Rightarrow$ local minimum.

Analyze Stationary Points using Eigenvalues

We analyze the eigenvalues of $\mathbf{H}$ at each stationary point: At $(0, 0)$:

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- Solving for λ yields $\lambda \approx 9.75$ and $\lambda \approx -3.75$. Result: Eigenvalues have mixed signs ($\lambda_1 > 0, \lambda_2 < 0$). The point $(0, 0)$ is a Saddle Point (Indefinite Hessian).

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- Solving for λ yields $\lambda \approx 15.65$ and $\lambda \approx 2.35$. All eigenvalues are positive. The point $(1, 1)$ is a Local Minimum (Positive Definite Hessian).

The Hessian Matrix and its Connection to the Lagrangian

The **Hessian matrix** $[H]$ of a scalar function $f(x_1, \ldots, x_N)$ is the square matrix of second-order partial derivatives:

$$[H]_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

In mechanical systems analysis, we use the Hessian of the potential energy function $V(\mathbf{x})$ at an equilibrium point $\mathbf{x}_{\text{eq}}$. This matrix describes the local curvature of the energy landscape and is essential for stability analysis.

The Connection to the Lagrangian

The connection is fundamental: the stiffness matrix $[K]$ derived via the Lagrangian method is precisely the Hessian of the potential energy component of the Lagrangian ($L = T - V$), evaluated at the equilibrium position.

$$[K] = [H]_V = \left[\begin{array}{ccc} \frac{\partial^2 V}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 V}{\partial x_1 \partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 V}{\partial x_N \partial x_1} & \cdots & \frac{\partial^2 V}{\partial x_N \partial x_N} \end{array} \right] \Bigg|_{\mathbf{x}=\mathbf{0}}$$

The Lagrangian provides the framework to define V, and the Hessian procedure provides the physical stiffness matrix $[K]$ used in the resulting equations of motion $[M]\ddot{\mathbf{x}} + [K]\mathbf{x} = \mathbf{0}$.

Taylor Expansion

Multivariate Taylor expansion:

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top (\mathbf{x} - \mathbf{x}_0) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^\top H(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0).$$

The Hessian provides the second-order term in the multivariate Taylor Series expansion around a point $\mathbf{x}_0$. This is crucial for numerical methods like Newton's Method for Optimization.

Potential Energy Expansion

For small displacements $\mathbf{q}$ around equilibrium:

$$V(\mathbf{q}) \approx V(0) + \tfrac{1}{2}\mathbf{q}^\top H \mathbf{q},$$

with H Hessian (force constant matrix).

Equations of Motion & Generalized Eigenvalue Problem

From Newton's second law:

$$M\ddot{\mathbf{q}} + H\mathbf{q} = 0 \quad \Rightarrow \quad H\mathbf{v} = \lambda M\mathbf{v},$$

where $\lambda = \omega^2$ and M is diagonal mass matrix.

Mass-Weighting Transformation

Define mass-weighted Hessian:

$$K_{ij} = \frac{H_{ij}}{\sqrt{m_i m_j}}.$$

Solve $K\mathbf{v}' = \lambda\mathbf{v}'$ to obtain eigenvalues and eigenvectors. We will derive in a straightforward way. Go to next slides.

Two-Mass System

https://phys.libretexts.org/Bookshelves/Classical_Mechanics/Classical_Mechanics_(Tatum)/17 :

Consider two masses m_1 and m_2 connected by two springs with constants k_1 and k_2 in a linear chain, with the ends fixed (e.g., k_1 connected to a wall, then m_1, then k_2, then m_2). Let q_1 and q_2 be the displacements from equilibrium. The total potential energy is:
$V(q_1, q_2) = \frac{1}{2}k_1 q_1^2 + \frac{1}{2}k_2(q_2 - q_1)^2$.

- Compute the Hessian : **H**:

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 V}{\partial q_1^2} & \frac{\partial^2 V}{\partial q_1 \partial q_2} \\ \frac{\partial^2 V}{\partial q_2 \partial q_1} & \frac{\partial^2 V}{\partial q_2^2} \end{pmatrix}$$

Two-mass systems: Hessian

- Here $\frac{\partial V}{\partial q_1} = k_1 q_1 - k_2(q_2 - q_1) \Rightarrow \frac{\partial^2 V}{\partial q_1^2} = k_1 + k_2$, $\frac{\partial V}{\partial q_2} = k_2(q_2 - q_1) \Rightarrow \frac{\partial^2 V}{\partial q_2^2} = k_2$, and $\frac{\partial^2 V}{\partial q_1 \partial q_2} = -k_2$.

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- Thus

$$\mathbf{H} = \begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{pmatrix}$$

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- Thus
$$\mathbf{H} = \begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{pmatrix}$$
- Form the Mass Matrix $\mathbf{M}$: $\mathbf{M} = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}$

Generalized Eigenvalue Problem

- Set up the Generalized Eigenvalue Problem:

$$\begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{pmatrix} \mathbf{v} = \lambda \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \mathbf{v}$$

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- We consider the symmetric case

$$k_1 = k_2 = k, \qquad m_1 = m_2 = m.$$

The stiffness matrix and mass matrix are

$$\mathbf{H} = \begin{pmatrix} 2k & -k \\ -k & k \end{pmatrix}, \qquad \mathbf{M} = \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix}.$$

Derivation

- Normal modes satisfy the generalized eigenvalue problem

$$\det(\mathbf{H} - \lambda \mathbf{M}) = 0, \qquad \lambda = \omega^2.$$

Thus,

$$\det \begin{pmatrix} 2k - m\omega^2 & -k \\ -k & k - m\omega^2 \end{pmatrix} = 0.$$

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- Expanding the determinant,

$$(2k - m\omega^2)(k - m\omega^2) - k^2 = 0,$$
$$m^2\omega^4 - 3km\omega^2 + k^2 = 0.$$

Let $x = \omega^2$. Then

$$m^2x^2 - 3km\,x + k^2 = 0.$$

Derivation

- Solving the quadratic,

$$x = \frac{3km \pm \sqrt{(3km)^2 - 4m^2k^2}}{2m^2}$$
$$= \frac{3k \pm k\sqrt{5}}{2m} = \frac{k}{m}\frac{3 \pm \sqrt{5}}{2}.$$

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- Thus the eigenvalues (squared frequencies) are

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- Numerically,

$$\omega_-^2 \approx 0.381966\,\frac{k}{m}, \qquad \omega_+^2 \approx 2.618034\,\frac{k}{m}.$$

Each corresponds to a specific geometric pattern of motion — a "dance move" the masses always follow if the system is started in that mode.

From

$$(2k - m\omega^2)A_1 - kA_2 = 0,$$

we obtain

$$\frac{A_2}{A_1} = 2 - \frac{m\omega^2}{k}.$$

Define

$$r = \frac{m\omega^2}{k} = \frac{3 \pm \sqrt{5}}{2}.$$

Then,

$$\frac{A_2}{A_1} = 2 - r = \frac{1 \mp \sqrt{5}}{2}.$$

Thus, the (unnormalized) eigenvectors are

$$\mathbf{A}_- \propto \begin{pmatrix} 1 \\ \dfrac{1+\sqrt{5}}{2} \end{pmatrix}, \qquad \mathbf{A}_+ \propto \begin{pmatrix} 1 \\ \dfrac{1-\sqrt{5}}{2} \end{pmatrix}.$$

Numerically,

$$\mathbf{A}_- \propto (1,\ 1.618), \qquad \mathbf{A}_+ \propto (1,\ -0.618).$$

Explanation

Interpretation: Frequencies and Mode Shapes

The resulting eigenvalues and eigenvectors carry the physical information:

- Eigenvalues (λ_i): They are directly related to the square of the angular frequency (ω) of vibration: $\lambda_i = \omega_i^2$.
  The vibrational frequency (ν) observed in spectroscopy is:

$$\nu_i = \frac{1}{2\pi}\sqrt{\lambda_i}.$$

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- Zero Eigenvalues ($\lambda_i = 0$): The system is not vibrating, it's just moving or rotating in space.

Explanation

Interpretation: Frequencies and Mode Shapes

- Negative Eigenvalues ($\lambda_i < 0$): These correspond to imaginary frequencies ($\nu_i \propto \sqrt{\text{negative number}}$). An imaginary frequency indicates that the geometry is a Saddle Point (a transition state in chemistry, or an unstable geometry in physics) and not a true local minimum.

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- For a chain of masses: Lowest mode ($j = 1$): masses move roughly together (in-phase) long-wavelength motion, lowest frequency Higher modes ($j = n$): masses alternate signs (out-of-phase), short-wavelength motion, highest frequency. Each higher mode introduces a "bend" or "node" in the motion

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- Eigenvectors ($\mathbf{v}_i$): Each eigenvector defines the Normal Mode Shape—the specific, collective motion of all atoms in that single, independent vibrational motion (e.g., a "symmetric stretch" or a "rocking" motion).

- Conclusion: The Hessian matrix transforms a complex, coupled system (a molecule) into uncoupled simple harmonic oscillators (the normal modes) by finding the optimal basis set (the eigenvectors) that diagonalizes the potential energy surface. This is a profound and essential application of matrix algebra in scientific computing.
- Normal modes are the fundamental vibration patterns of a system, each oscillating at its own natural frequency, and any motion is just a combination of these patterns.

Pseudocode for Matrix Generation

Assumes uniform mass m and stiffness k, fixed ends.

Listing 1: Generate Stiffness Matrix (K)

```
function Generate_K_Uniform(N, stiffness_k):
    K = zeros(N, N)
    for i from 0 to N-1:
        # Diagonal: Sum of adjacent springs (2k)
        K[i][i] = 2 * stiffness_k

        # Off-diagonal: Coupling (-k)
        if i > 0:
            K[i][i-1] = -stiffness_k
        if i < N-1:
            K[i][i+1] = -stiffness_k

    return K
```

Summary and Conclusion

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Hessian

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- Stability analysis