Thermodynamics and contact geometry Lecture 5: Differential invariants in thermodynamics

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July 23, 2021

Geometry of thermodynamics

We have during these lectures seen several geometric structures that are associated with thermodynamics.

Contact structure A thermodynamic system in equilibrium is a Legendrian submanifold of a contact manifold.

Metric The Legendrian submanifolds are equipped with a positive definite metric. Yesterday we saw that the measurement a point in the space V (modelled by a random vector) gave us Legendrian submanifolds of $V \times \mathbb{R} \times V^*$ endowed with a positive definite metric σ_2 . This metric was just the first of an infinite set of central moments.

A transformation on V induces a transformation on $V \times \mathbb{R} \times V^*$ by the requirement that it preserves the contact structure. The transformations on V that also preserve σ_2 are exactly the affine transformation on V.

In this lecture we will find the scalar differential invariants of Legendrian submanifolds under the group of affine transformations.

Differential invariants

Scalar differential invariants of geometric structures with respect to a group of transformations are functions that depend on the parameters of the structure and their derivatives and whose expressions do not change under the group action.

One example we saw yesterday was the scalar curvature of the metric $g = a(x,y)dx^2 + 2b(x,y)dxdy + c(x,y)dy^2$, which is a differential invariant with respect to the pseudogroup of local diffeomorphisms. It is given by

$$Sc = -\frac{a_{yy} - 2b_{xy} + c_{xx}}{ac - b^2} - \frac{(-aa_yc_y + 2ab_xc_y - ac_x^2 - ba_xc_y + 2ba_yb_y + ba_yc_x - 4bb_xb_y + 2bb_xc_x + 2ca_xb_y - ca_xc_x - ca_y^2)}{2(ac - b^2)^2}$$

If the group action signifies some arbitrary choice in our description of a physical system, the invariants are those quantities that are independent of this choice: They are the quantities of the underlying physics. This is illustrated well by the scalar curvature which in general relativity appears as a quantity that all observers agree upon.

A simple example

Let us illustrate the concept of differential invariants using one of the simplest possible examples.

The Euclidean plane is the space $\mathbb{R}^2(x,y)$ endowed with the group of rigid motions:

$$\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} a \\ b \end{pmatrix}$$

Let us consider the set $C^{\infty}(\mathbb{R}^2)$ of smooth functions on this space.

The transformation group induces an action on functions on the Euclidean plane, and two functions f and g can be considered to be equivalent if there exists a Euclidean transformation φ so that $f \circ \varphi = g$.

In order to determine when two functions are equivalent, we will find a set of invariant quantities, i.e. quantities that are not affected by the transformation.

Group-action on Taylor polynomials

The transformation group acts on the second-degree Taylor polynomial of $f \in C^{\infty}(\mathbb{R}^2)$,

$$[f]^{2}_{(x_{0},y_{0})} = a_{0} + a_{1}(x - x_{0}) + a_{2}(y - y_{0}) + \frac{a_{11}}{2}(x - x_{0})^{2} + a_{12}(x - x_{0})(y - y_{0}) + \frac{a_{22}}{2}(y - y_{0})^{2}.$$

The coefficients $a_0, a_1, ..., a_{22}$ depend on the point (x_0, y_0) . Using a translation from our group, we can transform the Taylor polynomial to

$$[f]_{(0,0)}^2 = a_0 + a_1 x + a_2 y + \frac{a_{11}}{2} x^2 + a_{12} x y + \frac{a_{22}}{2} y^2.$$

The only thing we can do now (without undoing the previous step) is to apply a rotation. We use it to remove the coefficient of x. Let

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} = \frac{1}{\sqrt{a_1^2 + a_2^2}} \begin{pmatrix} a_2 & a_1 \\ -a_1 & a_2 \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix}.$$

Then, we get the Taylor polynomial

$$a_0 + \sqrt{a_1^2 + a_2^2} \tilde{y} + \frac{a_2^2 a_{11} - 2a_1 a_2 a_{12} + a_1^2 a_{22}}{a_1^2 + a_2^2} \frac{\tilde{x}^2}{2} + \frac{(a_2^2 - a_1^2)a_{12} - a_1 a_2(a_{22} - a_{11})}{a_1^2 + a_2^2} \tilde{x} \tilde{y} + \frac{a_1^2 a_{11} + 2a_1 a_2 a_{12} + a_2^2 a_{22}}{a_1^2 + a_2^2} \frac{\tilde{y}^2}{2}$$

Extracting invariant functions

Note that a requirement for applying the last rotation was that $a_1^2 + a_2^2 > 0$.

The normalized coefficients of our Taylor polynomial,

$$\frac{a_0, \quad \sqrt{a_1^2 + a_2^2}, \quad \frac{a_2^2 a_{11} - 2a_1 a_2 a_{12} + a_1^2 a_{22}}{a_1^2 + a_2^2},}{a_1^2 + a_2^2},$$
$$\frac{(a_2^2 - a_1^2)a_{12} - a_1 a_2 (a_{22} - a_{11})}{a_1^2 + a_2^2}, \quad \frac{a_1^2 a_{11} + 2a_1 a_2 a_{12} + a_2^2 a_{22}}{a_1^2 + a_2^2}$$

can be considered as functions on the space of second-degree Taylor polynomials (the space of 2-jets). They are invariant.

Extracting invariant functions

Let us use the following invariants:

$$I_0 = a_0, \quad I_1 = a_1^2 + a_2^2, \quad I_{2a} = a_2^2 a_{11} - 2a_1 a_2 a_{12} + a_1^2 a_{22},$$

$$I_{2b} = (a_1^2 - a_2^2)a_{12} + a_1 a_2 (a_{22} - a_{11}), \quad I_{2c} = a_1^2 a_{11} + 2a_1 a_2 a_{12} + a_2^2 a_{22}$$

Since any algebraic combination of the invariants is invariant, they generate an algebra.

Recal that $a_0, a_1, a_2, a_{11}, ..., a_{22}$ depend on the point (x_0, y_0) , when f is fixed. In fact, we have

$$a_0 = f(x_0, y_0), \quad a_1 = f_x(x_0, y_0), \quad a_2 = f_y(x_0, y_0), \quad \dots, \quad a_{22} = f_{yy}(x_0, y_0).$$

The invariants depend on both the function f, and on (x_0, y_0) : If f is fixed, the invariants are functions on \mathbb{R}^2 . Let I_0^f, \dots, I_{2c}^f denote these functions on \mathbb{R}^2 .

Equivalence of functions

If two functions f_1 and f_2 are related by a Euclidean transformation, the functions $I_0^{f_1}$ and $I_0^{f_2}$ must be equivalent, and similarly for the other invariants.

For a generic function f, the functions $I_0^f(x, y), I_1^f(x, y)$ are independent functions of (x, y): $dI_0^f \wedge dI_1^f \neq 0$. Thus I_0^f and I_1^f can be used as (local) coordinates on \mathbb{R}^2 . The functions $I_{2a}^f, I_{2b}^f, I_{2c}^f$ can then be written in terms I_0^f, I_1^f :

$$I_{2a}^{f} = \alpha(I_{1}^{f}, I_{2}^{f}), \qquad I_{2b}^{f} = \beta(I_{1}^{f}, I_{2}^{f}), \qquad I_{2c}^{f} = \gamma(I_{1}^{f}, I_{2}^{f})$$

The functions α, β, γ are independent of the choice of representative in the equivalence class of f: If f_1 and f_2 are locally equivalent on a domain on which $I_0^{f_1}, I_1^{f_1}$ and $I_0^{f_2}, I_1^{f_2}$ serve as coordinates, they will determine the same functions α, β, γ .

Exercise: Consider the functions $f_1(x, y) = x^2 + y$ and $f_2(x, y) = x^2 - 2x + 1 + y$. Show that we have, for both of them, the relations

$$I_{2a} = 2,$$
 $I_{2b}^2 = 4(I_1 - 1),$ $I_{2c} = 2(I_1 - 1).$

Signature manifolds

Consider the two-dimensional submanifold in \mathbb{R}^5 parametrized by

$$(x,y) \mapsto \left(I_0^f(x,y), I_1^f(x,y), I_{2a}^f(x,y), I_{2b}^f(x,y), I_{2c}^f(x,y) \right).$$

We call it the signature manifold of f.

Equivalent functions give rise to the same signature manifolds. Conversely, if the invariants generate the whole algebra of invariants, then the signature manifold will also completely distinguish inequivalent functions. In this sense, the signature manifold solves the equivalence problem.

Important: Not all two-dimensional manifolds in \mathbb{R}^5 are realized as the signature of some function f, only those that satisfy a certain system of differential equations: The quotient PDE.

The differential algebra of differential invariants

Is it sufficient to consider only second-degree Taylor polynomials?

If we tried to normalize the third-degree Taylor polynomial of f, we would get four additional invariants, etc. It turns out that these can be generated by the previous ones. Not by algebraic operations, but by derivations.

Consider again the invariants restricted to the function f:

$$a = I_0^f, \quad b = I_1^f, \quad g = I_{2a}^f, \quad h = I_{2b}^f, \quad k = I_{2c}^f$$

Assume that $da \wedge db \neq 0$. Then a, b can be used as coordinates on \mathbb{R}^2 . Now we can differentiate g, h, k with respect to a and b to produce six new invariants. By continuing this, we can generate all invariants.

The quotient PDE

By differentiating g, h, k, we get 6 new invariants, but not all of these are independent. More concretely, we have

$$b^{2}h_{a} - 2bhk_{b} + 2bkh_{b} + (g+k)h = 0,$$

$$b^{2}g_{a} + 2bkg_{b} - 2bhh_{b} + g^{2} - 3gk + 4h^{2} = 0.$$

Notice that this holds for the invariants restricted to the function f. But they are actually independent of f.

We call this the quotient PDE. This is the PDE that the signature manifold must satisfy.

Measurements

Consider a random vector

 $X \colon (\Omega, \mathcal{A}, \mu_0) \to V$

where Ω is the sample space, ${\cal A}$ is the $\sigma\mbox{-algebra}$ of events, and μ_0 is a probability measure.

We interpret X as a measurement of $x_0 \in V$ if

$$E_{\mu_0}(X) = \int_{\Omega} X d\mu_0 = x_0.$$

Let us choose an affine frame such that $x_0 = 0$. The measurement of a vector $x \in V$ is given by a probability measure μ different from μ_0 , satisfying $E_{\mu}(X) = \int_{\Omega} X d\mu = x$. Assuming that μ is absolutely continuous with respect to μ_0 , we have by the Radon-Nikodym theorem $d\mu = \rho d\mu_0$.

Notice that E_{μ} behaves well under affine transformations:

$$E_{\mu}(AX + B) = AE_{\mu}(X) + B.$$

Constraints on ρ

We require

$$\int_{\Omega} \rho d\mu_0 = 1, \qquad E_{\mu}(X) = \int_{\Omega} \rho X d\mu_0 = x.$$

This is an underdetermined set of conditions on ρ . We define the information gain

$$I(\mu,\mu_0) = \int_{\Omega} \rho \ln \rho d\mu_0,$$

and require ρ to minimize $I(\mu, \mu_0)$. Jaynes noted that this (or more precisely the the maximation of entropy) is "the only unbiased assignment we can make". The three conditions imply

$$\rho = \frac{1}{Z(\lambda)} e^{\langle \lambda, X \rangle}$$

with $\lambda \in V^*$. Here λ is the (multidimensional) Lagrange multiplier for the proposed optimization problem. $Z(\lambda) = \int_{\Omega} e^{\langle \lambda, X \rangle} d\mu_0$ is called the partition function. Choosing basis on V gives us coordinates x^i on V, and dual coordinates λ_i on V^* .

Symplectic and contact structures

If we define $H(\lambda) = -\ln Z(\lambda)$, we get

$$H_{\lambda_i}(\lambda) = -\frac{1}{Z(\lambda)} Z_{\lambda_i}(\lambda) = -\int_{\Omega} X^i \frac{e^{\langle \lambda, X \rangle}}{Z(\lambda)} d\mu_0 = -x^i.$$

These *n* equations define an *n*-dimensional submanifold $L \subset V \times V^*$ which is Lagrangian with respect to symplectic form $dx^i \wedge d\lambda_i$. Restricting $I(\mu, \mu_0)$ to *L* gives

$$I(\lambda) = H(\lambda) + \langle \lambda, x \rangle = H(\lambda) - \lambda_i H_{\lambda_i}(\lambda).$$

Or if we can solve $H_{\lambda_i} = -x^i$ for $\lambda(x)$, we may write

 $I(x) = H(\lambda(x)) + \langle \lambda(x), x \rangle.$

And we notice that $I_{x^i} = \lambda_i$. This determines a Legendrian submanifold

$$\tilde{L} = \{u = I(x), \lambda_i = I_{x^i}(x)\} \subset V \times \mathbb{R} \times V^*$$

with respect to the contact form $du - \lambda_i dx^i$.

Invariant symmetric tensors

Central moments with respect to the extremal measure ρ corresponding to λ give additional structure on Legendrian submanifolds.

We write $X = X^i d\lambda_i$. The kth moment corresponds to a symmetric k-form:

$$m_{k} = \int_{\Omega} X^{\otimes k} \rho d\mu_{0} = \left(\int_{\Omega} X^{i_{1}} \cdots X^{i_{k}} \rho d\mu_{0} \right) d\lambda_{i_{1}} \otimes \cdots \otimes d\lambda_{i_{k}}$$
$$= \frac{Z_{\lambda_{i_{1}}} \cdots \lambda_{i_{k}}}{Z} d\lambda_{i_{1}} \otimes \cdots \otimes d\lambda_{i_{k}}$$

These are GL(V)-invariant, but not invariant under translations. The kth central moment (i.e. the moment of $X - m_1$) is given by

$$\sigma_k = \sum_{i=0}^k \binom{k}{i} m_i \cdot m_1^{(k-i)}.$$

They define Aff-invariant symmetric k-forms on Lagrangian manifolds, for $k \ge 2$.

Invariant symmetric tensors

If we use λ_i as coordinates on L (or \tilde{L}), we have

$$\sigma_2 = -H_{\lambda_i\lambda_j}d\lambda_i \otimes d\lambda_j = x^i_{\lambda_j}d\lambda_i \otimes d\lambda_j.$$

In the coordinates x^i it is given by

$$\sigma_2 = u_{x^i x^j} dx^i \otimes dx^j.$$

All the central moments are invariant under the group of affine transformations on V. We will use them to find scalar differential invariants. In the rest of this lecture, we will work with the Lagrangian submanifold $L \subset V \times V^*$. The only invariant we lose with this simplification is the one of order 0: u.

From invariant tensors to scalar invariants

We find an invariant frame on L and write the central moments in this frame. Then the coefficients are scalar invariants.

First we notice that $\alpha_1 = \lambda_i dx^i$ is invariant (since both du and $du - \lambda_i dx^i$ are). If we use coordinates λ_i on L, we may write $\alpha_1 = x^i_{\lambda_i} \lambda_i d\lambda_j$.

- σ_2 is nondegenerate, so we may construct a (second-order) invariant vector field $v_1 = \sigma_2^{-1}(\alpha_1)$.
- $\sigma_{1,3} = i_{v_1}\sigma_3$ is a symmetric 2-form. We use σ_2 to turn $\sigma_{1,3}$ into an operator $A: T \to T$.
- For $k \leq n$, let $v_i = A^{i-1}(v_1)$. They are independent on a generic Lagrangian manifold, and $\{v_1, ..., v_k\}$ is a frame of invariant vector fields (of third order).
- ▶ The functions $\sigma_k(v_{i_1}, ..., v_{i_k})$ are scalar differential invariants.

There is only one second-order invariant: $\sigma_2(v_1, v_1) = \lambda_i \lambda_j x_{\lambda_j}^i$. Note that all the invariants are rational functions.

The field of rational scalar differential invariants

Theorem

The set $\{\sigma_j(v_{i_1}, ..., v_{i_k}) \mid j = 2, ..., k\}$ contains a transcendence basis for the field of rational differential invariants of order k.

We have

$$i_{v_i}\sigma_2 = i_{v_{i-1}}i_{v_1}\sigma_3,$$

because of the way the frame was constructed. It implies relations

$$\sigma_3(v_1, v_i, v_j) = \sigma_3(v_1, v_{i+1}, v_{j-1}).$$

In two dimensions this holds trivially, since σ_3 is symmetric. In three dimensions we get the additional relation

$$\sigma_3(v_1, v_1, v_3) = \sigma_3(v_1, v_2, v_2).$$

The number of algebraically independent differential invariants of order k is summarized by the Hilbert function H_k :

$$H_1 = 0, \quad H_2 = 1, \quad H_3 = \frac{n^3 + 11n - 6}{6}, \quad H_k = \binom{n+k-1}{k}$$

The differential algebra

The vector fields v_i are derivations that act on the field of differential invariants and makes it a differential algebra.

Theorem

The differential algebra of differential invariants is generated by $v_1, ..., v_k$, and the scalar invariants $\sigma_2(v_1, v_1)$, $\sigma_3(v_i, v_j, v_k)$ and $\sigma_4(v_i, v_j, v_k, v_l)$.

If $\dim V = 2$, the third-order invariants are sufficient to generate the algebra. We simplify notation:

$$\begin{split} I_{21} &= \sigma_2(v_1, v_1), \quad I_{22} = \sigma_2(v_1, v_2), \quad I_{23} = \sigma_2(v_2, v_2), \quad I_{31} = \sigma_3(v_1, v_1, v_1), \\ I_{32} &= \sigma_3(v_1, v_1, v_2), \quad I_{33} = \sigma_3(v_1, v_2, v_2), \quad I_{34} = \sigma_3(v_2, v_2, v_2) \end{split}$$

And define

$$J_1 = \frac{I_{21}I_{33} - I_{22}I_{32}}{I_{21}I_{23} - I_{22}^2}, \quad J_2 = \frac{I_{22}I_{33} - I_{23}I_{32}}{I_{21}I_{23} - I_{22}^2}, \quad J_3 = \frac{I_{21}I_{34} - I_{22}I_{33}}{I_{21}I_{23} - I_{22}^2}, \quad J_4 = \frac{I_{22}I_{34} - I_{23}I_{33}}{I_{21}I_{23} - I_{22}^2}.$$

They can be expressed in terms of $I_{21}, I_{33}, I_{34}, v_1(I_{21})$ and $v_2(I_{21})$.

Generators and syzygies in 2D

Theorem

The differential algebra of scalar differential invariants is generated by the invariant derivations v_1 and v_2 , and the scalar differential invariants I_{21} , I_{33} and I_{34} . The differential syzygies are generated by

$$\begin{aligned} & 3J_4 \, v_1(v_1(I_{21})) - (2J_1 + 2J_2 + 3J_3) \, v_2(v_1(I_{21})) + J_1 \, v_2(v_2(I_{21})) - v_2(I_{33}) + v_1(I_{34}) \\ & -(4J_2 + 6J_4) \, v_1(I_{21}) + (4J_1 + 6J_2 + 6J_3) \, v_2(I_{21}) - J_2I_{33} + (4 + 2J_1)I_{34} + 8J_2I_{21} = 0, \\ & -4J_2 \, v_1(v_1(I_{21})) + (4J_1 - 2) \, v_2(v_1(I_{21})) + v_2(v_2(I_{21})) - 2 \, v_1(I_{33}) + I_{34} - 4J_1I_{33} \\ & +(8J_1 - 2J_1^2 + 6J_2) \, v_1(I_{21}) + (4J_2 - 12J_1 + 4) \, v_2(I_{21}) + (4J_1^2 + 2J_1J_2 + 4J_2 - 16J_1)I_{21} = 0. \end{aligned}$$

Application to thermodynamics

Let us use the following variables:

•
$$e = x^1$$
 - internal energy

 \blacktriangleright $v = x^2$ - volume

- $\blacktriangleright s = -I + C$ entropy
- \blacktriangleright $T = -1/\lambda_1$ temperature

•
$$p=\lambda_2/\lambda_1$$
 - pressure

$$\theta = du - \lambda_1 dx^1 - \lambda_2 dx^2 = -(ds - \frac{1}{T}de - \frac{p}{T}dv)$$

- By considering a measurement of (e, v), we identify the fundamental thermodynamic relation with the contact form arising in the context of measurements.
- A thermodynamic system in equilibrium corresponds to a Legendrian submanifold of (V × ℝ × V^{*}, θ), or a Lagrangian submanifold of (V × V^{*}, dθ).

Scalar differential invariants

Lagrangian submanifolds are given by two functions e(T,p), v(T,p), satisfying $Tv_T + pv_p + e_p = 0.$

Theorem

The algebra of scalar differential invariants is generated by the following differential invariants and invariant derivations:

$$I_{2} = pv_{T} + e_{T}, \qquad I_{31} = \nabla_{1}(I_{2}), \qquad I_{32} = \frac{(e_{T}v_{TT} - e_{TT}v_{T})^{2}T^{3}}{e_{p}v_{T} - e_{T}v_{p}},$$

$$I_{33} = \frac{(2Tv_{T}I_{2}v_{TT} + I_{2}^{2}v_{Tp} + v_{T}I_{31} + v_{T}^{2}I_{2})T}{(e_{p}v_{T} - e_{T}v_{p})^{2}},$$

$$I_{34} = \frac{T^{2}(3T^{2}v_{T}^{2}I_{2}v_{TT} + 3Tv_{T}I_{2}^{2}v_{Tp} + I_{2}^{3}v_{pp} + Tv_{T}^{3}I_{31} + 4Tv_{T}^{3}I_{2} + 3v_{T}v_{p}I_{2}^{2})(e_{T}v_{TT} - e_{TT}v_{T})}{(e_{p}v_{T} - e_{T}v_{p})^{2}},$$

$$\nabla_{1} = -TD_{T}, \qquad \nabla_{2} = \frac{Tv_{T}D_{T} + (e_{T} + pv_{T})D_{p}}{(e_{T}v_{TT} - e_{TT}v_{T})T}$$

Heat capacity

The concept of heat capacity plays an important role in thermodynamics. It is commonly defined as

$$C = \lim_{\Delta T \to 0} \frac{Q}{\Delta T},$$

where ${\cal Q}$ is the heat added to the system. Keeping the pressure p fixed gives the "heat capacity at constant pressure"

$$C_p = e_T + pv_T$$

which is the simplest of our differential invariant.

Example. Gases with constant heat capacity:

$$e(T,p) = f_1(p)T - f'_2(p)p^2, \quad v(T,p) = \frac{(C_p - f_1(p))T}{p} + f'_2(p)p + f_2(p)$$

Differential invariants for a subgroup appearing in fluid dynamics

Inspired by [Duyunova et. al. 2017] we consider the group action given by $(e,v) \mapsto (Ae + Cv, Bv)$ for $A, B \in \mathbb{R} \setminus \{0\}, C \in \mathbb{R}$ which appears in the study of fluids. It is a subgroup of the group of affine transformations, meaning that there are more invariants.

Theorem

The following is a transcendence basis for the field of rational differential invariants of order 2:

$$\frac{e+pv}{T}, \qquad \frac{Tv_T}{v}, \qquad C_p = e_T + pv_T, \qquad C_v = e_T - e_p \frac{v_T}{v_p}$$

We note that e + pv is the enthalpy, v_T/v is the coefficient of thermal expansion, C_p is the heat capacity at constant pressure and C_v is the heat capacity at constant volume.

Differential invariants for a subgroup appearing in fluid dynamics

Theorem

The differential algebra of differential invariants is generated by

$$J_1 = \frac{e + pv}{T}, \qquad J_2 = \frac{Tv_p}{v^2}, \qquad \tilde{\nabla}_1 = TD_T, \qquad \tilde{\nabla}_2 = \frac{T}{v}D_p.$$

These generators are related by the differential syzygy

$$\tilde{\nabla}_1(J_2) + \tilde{\nabla}_2(\tilde{\nabla}_2(J_1)) - J_2\tilde{\nabla}_2(J_1) = 0.$$

Example: The thermodynamic systems for which J_1 is constant are given by

$$e = (C_1 - f(p))T, \qquad pv = f(p)T.$$

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