Dynamical distribution networks: power networks

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Power networks as an example of dynamical distribution networks

- Dynamical distribution networks appear in many areas of engineering and natural sciences:
  power networks, gas and heat distribution networks, metabolic reaction networks, ...
  'Classical' examples like electrical circuits, mechanical networks, ...
- Sometimes with additional dynamical network layers: control and communication networks, gene-regulatory networks, ..
- Dynamical distribution networks typically operate under non-zero inflow and outflow, 'out of equilibrium', ...
  As a result, natural candidates for stability analysis such as total energy cannot be used as Lyapunov function.
- They are often large-scale: scalable theory is needed.
- Underlying geometry is determined by network ('incidence') structure.

Outline

Basic background on graphs

Directed graph with N nodes, and M edges.

Specified by its $N \times M$ incidence matrix D,
each column corresponds to an edge, with -1 for tail node and 1 for head node; 0 otherwise.

Basic property

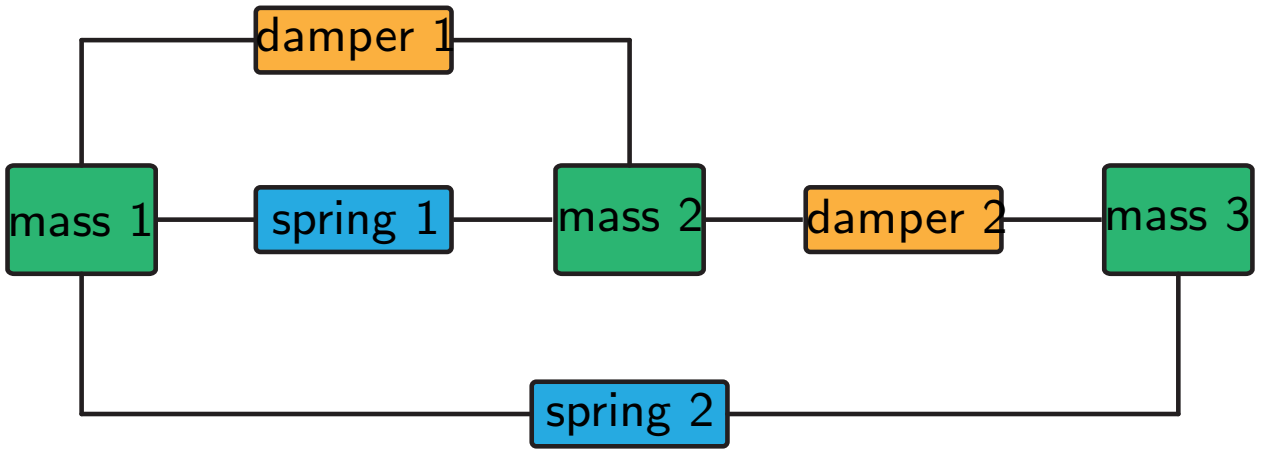
$$\mathbb{1}^T D = 0\,,$$

where $\mathbb{1}$ is the vector of all ones.

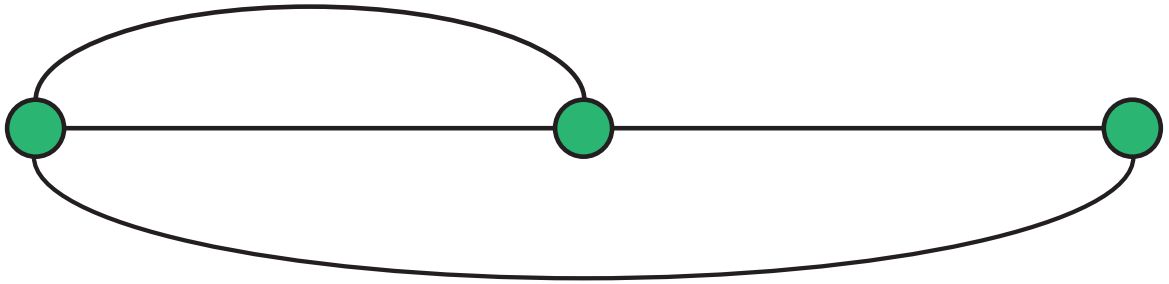
$\ker D^T = \operatorname{span} \mathbb{1}$ if and only if the graph is connected
(which will be assumed, without loss of generality, throughout).

On the other hand, $\ker D$ is the space of cycles.

Associate masses to nodes, and springs and dampers to edges.



(a)



(b)

$$D = \begin{bmatrix} D_s & | & D_d \end{bmatrix} = \left[\begin{array}{cc|cc} -1 & -1 & -1 & 0 \\ 1 & 0 & 1 & -1 \\ 0 & 1 & 0 & 1 \end{array}\right]$$

Dynamics is Hamiltonian plus energy-dissipation:

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \left(\begin{bmatrix} 0 & D_s^T \\ -D_s & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & D_d R D_d^T \end{bmatrix} \right) \begin{bmatrix} \frac{\partial H}{\partial q}(q,p) \\ \frac{\partial H}{\partial p}(q,p) \end{bmatrix}$$

$D_d R D_d^T$ is Laplacian matrix, with R diagonal matrix of damping constants.

Hamiltonian in the linear case

$$H(q,p) = \frac{1}{2} p^T M^{-1} p + \frac{1}{2} q^T K q$$

M mass matrix, K spring matrix.

Compositional point of view !

Some analysis

Proposition

Set of equilibria $\mathcal{E}$ is

$$\mathcal{E} = \{(q,p) \mid \frac{\partial H}{\partial q}(q,p) \in \ker D_s,\ v = \frac{\partial H}{\partial p}(q,p) \in \operatorname{span} \mathbb{1}\}$$

Proposition

Casimir functions (conserved quantities independent of H) are all functions $C(q,p)$ satisfying

$$\frac{\partial C}{\partial p}(q,p) \in \operatorname{span} \mathbb{1}, \quad \frac{\partial C}{\partial q}(q,p) \in \ker D_s,$$

which can be expressed as functions of elementary Casimirs

$$C(p) = \mathbb{1}^T p, \quad C(q) = c^T q, \quad c \in \ker D_s \quad \textit{(cycles)}$$

Hence, starting from any initial position (q_0, p_0) the solution will be contained in

$$\mathcal{A}_{(q_0,p_0)} := \begin{bmatrix} q_0 \\ p_0 \end{bmatrix} + \begin{bmatrix} 0 \\ \ker \mathbb{1}^T \end{bmatrix} + \begin{bmatrix} \operatorname{im} D_s^T \\ 0 \end{bmatrix}$$

Theorem

Define the spring Laplacian matrix $L_s := D_s K D_s^T$.

Then for every (q_0, p_0) *there exists a unique equilibrium point*

$$(q_\infty, p_\infty) \in \mathcal{E} \cap \mathcal{A}_{(q_0,p_0)},$$

to which the system converges exponentially if and only if the largest $M^{-1}L_s$*-invariant subspace contained in* $\ker L_d$ *equals* $\operatorname{span} \mathbb{1}$.

Can be extended to nonlinear case.

Mass-spring-damper systems with external forces

Port-Hamiltonian system

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & D_s^T \\ -D_s & -D_d R D_d^T \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q}(q,p) \\ \frac{\partial H}{\partial p}(q,p) \end{bmatrix} + \begin{bmatrix} 0 \\ E \end{bmatrix} u$$

$$y = \begin{bmatrix} 0 & E^T \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q}(q,p) \\ \frac{\partial H}{\partial p}(q,p) \end{bmatrix}$$

with u the external forces acting on the actuated masses, and y their velocities.

Steady-state analysis for constant $\bar{u}$

Assume existence of $\bar{q}$ s.t.

$$D_s \frac{\partial H}{\partial q}(\bar{q}, 0) = \bar{u}$$

(*spring forces can compensate for external forces*)
Define shifted Hamiltonian (or availability function)

$$\widehat{H}(q,p) := H(q,p) - \frac{\partial H}{\partial q^T}(\bar{q},0)(q-\bar{q}) - H(\bar{q},0)$$

System can be rewritten as

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & D_s^T \\ -D_s & -D_d R D_d^T \end{bmatrix} \begin{bmatrix} \frac{\partial \widehat{H}}{\partial q}(q,p) \\ \frac{\partial \widehat{H}}{\partial p}(q,p) \end{bmatrix}$$

If H is convex then $\widehat{H}$ has minimum at $(\bar{q}, 0)$.

Outline

Operation of electricity network is changing:

from a top-down network, distributing power from a few large generators to many loads, towards a multi-agent distribution network; with additional communication layers.

- Increasing share of renewable energy sources with large variability; consumers becoming 'prosumers'; distributed control instead of 'top-down'; ...
- All kinds of possibilities and needs for communication between generating and consuming units; 'smart grids'.
- Fundamental open stability questions; some classical, others by changing operation near limits of capacity, and caused by additional communication and market dynamics.

Simplest dynamical model: swing equation model

Underlying assumptions:

- All voltages and currents across/through the transmission lines (edges) are pure sinusoids with same frequency $\widehat{\omega}$ (50 Hz). Hence, any voltage (or, current) signal

$$V(t) = V \sin(\widehat{\omega} t + \phi), \quad t \in \mathbb{R},$$

  can be represented by its phasor

$$V e^{j\phi} \in \mathbb{C}$$

- Amplitudes V_i of voltage potentials at all n nodes are constant.
- All lines are purely inductive (phase shift of 90 degrees).

Power networks modeled by swing equations

Model any i-th generator (or synchronous machine) as a voltage source with voltage angle δ_i, with its reactance included into the transmission line.
Average power ('active power') flow through the k-th line from node i to node j is

$$\Gamma_k \sin(\delta_i - \delta_j)$$

with $\Gamma_k = S_k V_i V_j$, S_k susceptance of the line.
Define phase differences across the k-th line between node i and j

$$q_k := \delta_j - \delta_i, \qquad \text{i.e., } q = D^T \delta,$$

with D the $n \times m$ incidence matrix of the network:
Vector of power flows through the lines is

$$P = -D\Gamma \operatorname{Sin} D^T \delta = -D\Gamma \operatorname{Sin} q$$

where $\operatorname{Sin} : \mathbb{R}^m \to \mathbb{R}^m$ is the element-wise sin function.

Let ω_i be frequency deviation with respect to $\widehat{\omega}$ (50Hz) of node i.
Balance between mechanical and electrical nodal power flows

$$M\dot{\omega} = -A\omega + P + u = -A\omega - D\Gamma \operatorname{Sin} q + u, \quad \omega = (\omega_1, \cdots, \omega_n)^T$$

where $u \in \mathbb{R}^n$ is vector of produced/consumed power at nodes, and $A\omega$ is vector of damping torques, with A positive diagonal matrix.

Vector of phase differences $q = D^T\delta$ satisfies

$$\dot{q} = D^T\dot{\delta} = D^T\omega$$

Together, we obtain the swing equation network model

$$\begin{aligned} \dot{q} &= D^T\omega \\ M\dot{\omega} &= -A\omega - D\Gamma \operatorname{Sin} q + u \end{aligned}$$

Favorite equations in the control literature on power networks.

Swing equation model is port-Hamiltonian:

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & D^T \\ -D & -A \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q}(q,p) \\ \frac{\partial H}{\partial p}(q,p) \end{bmatrix} + \begin{bmatrix} 0 \\ I \end{bmatrix} u, \quad p = M\omega$$

$$y = \begin{bmatrix} 0 & I \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial q}(q,p) \\ \frac{\partial H}{\partial p}(q,p) \end{bmatrix} = \omega$$

with q phase differences across the lines, ω frequency deviations, $p = M\omega$ momentum deviations at the nodes, and u generated/consumed power.

Hamiltonian

$$H(q,p) = \frac{1}{2} p^T M^{-1} p - \sum_k \gamma_k \cos q_k$$

with γ_k constant of k-th line

Stability analysis for constant power in/outflow

Let $\bar{u}$ be a constant input, yielding steady state values $(\bar{q}, \bar{p} = M\bar{\omega})$.

Then $D^T\bar{\omega} = 0$ and thus by connectivity

$$\bar{\omega} = \mathbb{1}\omega_*, \quad \omega_* \in \mathbb{R} \text{ common frequency deviation}$$

Furthermore

$$\mathbb{1}^T A \mathbb{1}\omega_* = \mathbb{1}^T \bar{u}, \qquad \text{hence} \qquad \omega_* = \frac{\mathbb{1}^T \bar{u}}{\mathbb{1}^T A \mathbb{1}},$$

and

$$D\frac{\partial H}{\partial q}(\bar{q}) = -A\mathbb{1}\omega_* + \bar{u}$$

In particular $\omega_* = 0$ (zero frequency deviation) if and only if $\mathbb{1}^T\bar{u} = 0$

(*total consumed power = total generated power*).

Similar to mass-spring-damper case; however, all edges correspond to 'nonlinear springs', and 'dampers' are at the nodes.
Consequently, unique steady state (if any).

Define again availability function

$$\widehat{H}(q,p) := \frac{1}{2}(p-\bar{p})^T M^{-1}(p-\bar{p}) - \sum_k \gamma_k \cos q_k + \sum_k \gamma_k \sin \bar{q}_k \,(q_k - \bar{q}_k)$$

having strict minimum at $(\bar{q},\bar{p})$, whenever $\bar{q} \in (-\frac{\pi}{2},\frac{\pi}{2})^n$.

Then the system can be rewritten as

$$\begin{bmatrix}\dot{q}\\ \dot{p}\end{bmatrix} = \begin{bmatrix}0 & D^T\\ -D & -A\end{bmatrix}\begin{bmatrix}\frac{\partial \widehat{H}}{\partial q}(q,p)\\ \frac{\partial \widehat{H}}{\partial p}(q,p)\end{bmatrix} + \begin{bmatrix}0\\ I\end{bmatrix}(u-\bar{u})$$

$$y - \bar{y} = \frac{\partial \widehat{H}}{\partial p}(q,p)$$

and satisfies shifted energy balance

$$\frac{d}{dt}\widehat{H}(x(t)) \leq (u(t)-\bar{u})^T (y(t)-\bar{y})$$

Hence for $u = \bar{u}$ steady state $(\bar{q},\bar{p} = M\omega_*)$ is asymptotically stable.

Outline

Write $u = u_g - u_d$, with u_g generated power and u_d consumed power.

Maximize the social welfare function

$$U(u_d) - C(u_g),$$

with concave utility function $U(u_d)$ of the consumers u_d,
and convex generation cost $C(u_g)$ of the producers u_g,
under the constraint of zero frequency deviation.

Recall 'iff' condition for zero frequency deviation:

$$\mathbb{1}^T u_d = \mathbb{1}^T u_g$$

Furthermore, (u_g, u_d) satisfies this equation iff there exists $v \in \mathbb{R}^{m_c}$ such that

$$D_c v - u_g + u_d = 0,$$

where $D_c \in \mathbb{R}^{n \times m_c}$ is the incidence matrix of an arbitrary connected communication graph with same nodes.

Leads to convex minimization problem:

$$\begin{aligned} \min_{u_g, u_d, v} \quad & C(u_g) - U(u_d) \\ \text{s.t.} \quad & D_c v - u_g + u_d = 0 \end{aligned}$$

Corresponding Lagrangian is

$$L = C(u_g) - U(u_d) + \lambda^T (D_c v - u_g + u_d)$$

with Lagrange multipliers $\lambda \in \mathbb{R}^n$. The KKT optimality conditions ($\nabla L = 0$) are

$$\begin{aligned} \nabla C(\bar{u}_g) - \bar{\lambda} &= 0 \\ -\nabla U(\bar{u}_d) + \bar{\lambda} &= 0 \\ D_c^T \bar{\lambda} &= 0 \\ D_c \bar{v} - \bar{u}_g + \bar{u}_d &= 0. \end{aligned}$$

λ_i represents price at i-th node, and elements of v represent information exchange of the differences of the prices along the edges the communication graph.

Dynamic pricing controller

A continuous-time algorithm to converge to saddle-point described by the KKT conditions is steepest descent/ascent gradient dynamics

$$\begin{aligned}\tau_g \dot{u}_g &= -\nabla C(u_g) + \lambda + w_g \\ \tau_d \dot{u}_d &= \nabla U(u_d) - \lambda + w_d \\ \tau_v \dot{v} &= -D_c^T \lambda \\ \tau_\lambda \dot{\lambda} &= D_c v - u_g + u_d\end{aligned}$$

with time-scale matrices

$$\tau_g, \tau_d, \tau_v, \tau_\lambda > 0$$

Admits natural port-Hamiltonian formulation: define new state variables

$$x_g = \tau_g u_g,\ x_d = \tau_d u_d,\ x_v = \tau_v v,\ x_\lambda = \tau_\lambda \lambda$$

with quadratic Hamiltonian (see Arrow & Hurwicz, 1958)

$$H_m(x) = \frac{1}{2} x_g^T \tau_g^{-1} x_g + \frac{1}{2} x_d^T \tau_d^{-1} x_d + \frac{1}{2} x_v^T \tau_v^{-1} x_v + \frac{1}{2} x_\lambda^T \tau_\lambda^{-1} x_\lambda$$

$$\dot{x} = \begin{bmatrix} 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & -I \\ 0 & 0 & 0 & -D_c^T & -D_c^T \\ -I & 0 & D_c & 0 & 0 \\ 0 & I & D_c & 0 & 0 \end{bmatrix} \nabla H_m(x) + \frac{\partial W}{\partial z}(\nabla H_m(x)) + \begin{bmatrix} I & 0 \\ 0 & I \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v_g \\ v_l \end{bmatrix}$$

$$\begin{bmatrix} w_g \\ w_l \end{bmatrix} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \end{bmatrix} \nabla H_m(x)$$

Result: dynamic pricing controller. To be connected to the power network.

Using the sum of the shifted versions of H (power network) and H_m (market dynamics) leads to overall asymptotic stability of combined dynamics.

Outline

CRN theory; Horn, Jackson, Feinberg, Othmer, $\cdots$

Dynamics of r reactions among m chemical species with concentrations $x \in \mathbb{R}^m_+$ is

$$\dot{x} = Sv(x)$$

with reaction rate $v(x)$, and S the $m \times r$ stoichiometric matrix, which can be factorized as

$$S = ZD$$

with Z the $m \times c$ complex composition matrix and D the incidence matrix of the graph of complexes. For example

$$X_1 + 2X_2 \rightleftharpoons X_3 \rightleftharpoons 2X_1 + X_2$$

$$S = \begin{bmatrix} -1 & 2 \\ -2 & 1 \\ 1 & -1 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 & 2 \\ 2 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad D = \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}$$

Mass action kinetics of j-th reaction, from substrate complex $\mathcal{S}$ to product complex $\mathcal{P}$, prescribes

$$v_j(x) = k_j^+ \prod_{i=1}^{m} x_i^{Z_{i\mathcal{S}}} - k_j^- \prod_{i=1}^{m} x_i^{Z_{i\mathcal{P}}},$$

where $Z_{i\mathcal{S}}$ is the (i,ρ)-th element of the complex composition matrix Z, and k_j^+, k_j^- are the forward/backward reaction constants.
Can be rewritten as

$$v_j(x) = k_j^+ \exp\left(Z_{\mathcal{S}}^T \mathrm{Ln}(x)\right) - k_j^- \exp\left(Z_{\mathcal{P}}^T \mathrm{Ln}(x)\right)$$

Network is detailed balanced if there exists x^* satisfying

$$v(x^*) = 0$$

that is,

$$k_j^+ \exp\left(Z_{\mathcal{S}}^T \mathrm{Ln}(x^*)\right) = k_j^- \exp\left(Z_{\mathcal{P}}^T \mathrm{Ln}(x^*)\right), \quad j = 1, \cdots, r$$

Defining equilibrium constants

$$K_j^{eq} := \frac{k_j^+}{k_j^-}$$

this means

$$K^{eq} = \mathrm{Exp}\left(D^T Z^T \mathrm{Ln}\left(x^*\right)\right) = \mathrm{Exp}\left(S^T \mathrm{Ln}\left(x^*\right)\right),$$

where K^{eq} is the r-dimensional vector with j-th element K_j^{eq}.

Hence, the network is detailed balanced, if and only if

$$\mathrm{Ln}\left(K^{eq}\right) \in \mathrm{im}\, S^T$$

(generalized Wegscheider conditions)

Port-Hamiltonian formulation

Define conductance of j-th reaction as

$$\kappa_j(x^*) := k_j^+ \exp\left(Z_{\mathcal{S}}^T \mathrm{Ln}(x^*)\right) = k_j^- \exp\left(Z_{\mathcal{P}}^T \mathrm{Ln}(x^*)\right)$$

Then

$$v_j(x) = \kappa_j(x^*)\left[\exp\left(Z_{\mathcal{S}}^T \mathrm{Ln}\left(\frac{x}{x^*}\right)\right) - \exp\left(Z_{\mathcal{P}}^T \mathrm{Ln}\left(\frac{x}{x^*}\right)\right)\right]$$

Defining the $r \times r$ diagonal matrix of conductances $\mathcal{K}$ it follows that

$$v(x) = -\mathcal{K} D^T \mathrm{Exp}\left(Z^T \mathrm{Ln}\left(\frac{x}{x^*}\right)\right),$$

and thus the dynamics takes the form

$$\dot{x} = -Z\mathcal{L}\,\mathrm{Exp}\left(Z^T \mathrm{Ln}\left(\frac{x}{x^*}\right)\right)$$

with $\mathcal{L} := D\mathcal{K}D^T$ Laplacian matrix of the graph of complexes.

Fundamental property: for any $\gamma \in \mathbb{R}^c$

$$\gamma^T \mathcal{L} \operatorname{Exp} \gamma \geq 0,$$

with equality if and only if $D^T \gamma = 0$.

Yields easy proofs for a number of key results in CRN theory:

Property 1:
All positive equilibria are in fact detailed-balanced equilibria, and given one detailed-balanced equilibrium x^* the set of all positive equilibria is

$$\mathcal{E} := \{x^{**} \in \mathbb{R}^m_+ \mid S^T \operatorname{Ln} x^{**} = S^T \operatorname{Ln} x^*\}$$

Property 2:
There exists for any initial condition $x_0 \in \mathbb{R}^m_+$ unique steady state $x^{**} \in \mathcal{E}$ such that $x^{**} - x_0 \in \operatorname{im} S$.

Property 3:

Define

$$G(x) := x^T \mathrm{Ln}\left(\frac{x}{x^*}\right) + (x^* - x)^T \mathbb{1}_m$$

Since $\frac{\partial G}{\partial x}(x) = \mathrm{Ln}\left(\frac{x}{x^*}\right) =: \mu(x)$, it follows that the dynamics can be also written as

$$\dot{x} = -Z\mathcal{L}\,\mathrm{Exp}\left(Z^T \frac{\partial G}{\partial x}(x)\right)$$

Hence

$$\frac{d}{dt}G = -\mu^T(x)Z^T\mathcal{L}\,\mathrm{Exp}\,(Z^T\mu(x)) = -\gamma^T(x)\mathcal{L}\,\mathrm{Exp}\,\gamma(x) \leq 0$$

It follows that the vector of concentrations $x(t)$ starting from x_0 will converge for $t \to \infty$ to x^{**} if the reaction network is assumed to be persistent (no convergence to the boundary of the positive orthant $\mathbb{R}^m_+$).

Up to a constant G equals the Gibbs' free energy, while

$$\frac{\partial G}{\partial x}(x) = \mathrm{Ln}\left(\frac{x}{x^*}\right)$$

equals the vector of chemical potentials. The dynamics

$$\dot{x} = -Z\mathcal{L}\,\mathrm{Exp}\left(Z^T\frac{\partial G}{\partial x}(x)\right)$$

can be interpreted as arising from terminating the auxiliary i/o system

$$\begin{aligned}\dot{x} &= Zu\\ y &= Z^T\frac{\partial G}{\partial x}(x)\end{aligned}$$

with the energy-dissipating relation

$$u = -\mathcal{L}\,\mathrm{Exp}\,y,$$

and thus defines a port-Hamiltonian system with Hamiltonian G ('nonlinear mass-damper system').

Mass action networks with non-zero inflows and outflows

Metabolic reaction networks always have inflows and outflows of chemical species. Typically no constant outflows of species.

Horn: add extra zero complex: edges from the zero complex model the constant inflows into the network, while the edges towards the zero complex model mass action kinetics outflows.

Theorem

Assume x^* is complex-balanced equilibrium of extended reaction network:

$$D_e v_e(x^*) = 0$$

If each component is connected to zero complex, then set of steady states

$$\mathcal{E} = \{x^{**} \in \mathbb{R}^m_+ \mid Z^T \operatorname{Ln} x^{**} = Z^T \operatorname{Ln} x^*\}$$

For every $x_0 \in \mathbb{R}^m_+$, there exists unique $x_1 \in \mathcal{E}$ with $x_1 - x_0 \in \operatorname{im} S$, asymptotically stable with respect to those initial conditions x_0.

Outline

- Dynamical distribution networks are naturally modeled as port-Hamiltonian systems, with geometry determined by network.
- Distribution networks typically have non-zero inflows and outflows.
- Shifted Hamiltonian can be used as Lyapunov function for constant in/outflows in case of mass-spring-damper systems and swing equation model of power networks.
  Holds in general, if Poisson structure is constant, energy dissipation is linear and constant, and Hamiltonian is convex.
- Dynamic pricing controller combines stable physical network dynamics with optimization; all within a port-Hamiltonian framework.
- Closed chemical reaction networks are typically detailed-balanced, in which case the dynamics is like non-linear mass-damper system.
- General picture for chemical reaction networks with inflows and outflows unclear !
- How to combine the dynamical distribution network with other dynamical layers ?
  E.g., metabolic reaction network catalyzed by enzymes controlled by gene regulatory network.

Outline

Famous quote on classical, macroscopic, thermodynamics taken from Albert Einstein's autobiographical notes:

A theory is more impressive the greater the simplicity of its premises, the more different things it relates, and the more extended its area of applicability. Hence the deep impression that classical thermodynamics made upon me.
It is the only physical theory of universal content concerning which I am convinced that, within the framework of the applicability of its basic concepts, it will never be overthrown.

Thermodynamics is especially interesting for systems and control, since it directly originates in engineering (maximal efficiency of steam engines, ..), and always considers systems in interaction with others.

At the same time, thermodynamics is a somewhat confusing subject; and not always clearly presented ...

Outline

Consider two heat compartments with conducting wall. The two systems, indexed by 1 and 2, exchange heat flow q given by Fourier's law

$$q = \lambda(T_1 - T_2),$$

with temperatures

$$T_i = \frac{\partial U_i}{\partial S_i}(S_i), \quad i = 1, 2,$$

with $U_1(S_1), U_2(S_2)$ internal energies of two compartments.

Leads to pseudo port-Hamiltonian system

$$\begin{bmatrix} \dot{S}_1 \\ \dot{S}_2 \end{bmatrix} = \begin{bmatrix} -\frac{q}{T_1} \\ \frac{q}{T_2} \end{bmatrix} = \begin{bmatrix} -\lambda\frac{T_1 - T_2}{T_1} \\ \lambda\frac{T_1 - T_2}{T_2} \end{bmatrix} = \begin{bmatrix} 0 & \lambda(\frac{1}{T_1} - \frac{1}{T_2}) \\ -\lambda(\frac{1}{T_1} - \frac{1}{T_2}) & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial U}{\partial S_1} \\ \frac{\partial U}{\partial S_2} \end{bmatrix}$$

with total energy $U(S_1, S_2) := U_1(S_1) + U_1(S_2)$.

Pseudo port-Hamiltonian, since the skew-symmetric map

$$\begin{bmatrix} 0 & \lambda(\frac{1}{T_1} - \frac{1}{T_2}) \\ -\lambda(\frac{1}{T_1} - \frac{1}{T_2}) & 0 \end{bmatrix}$$

does not depend on S_1, S_2 directly, but through $T_i = \frac{\partial U_i}{\partial S_i}(S_i)$.

Therefore does not define Dirac structure on state space $\mathbb{R}^2$ with coordinates S_1, S_2: mixing of interconnection and constitutive relations.

Instead, example of the type

$$\dot{x} = J(e)e, \quad J(e) = -J^T(e), \quad e = \frac{\partial H}{\partial x}(x)$$

As a consequence

$$\dot{S}_1 + \dot{S}_2 = \frac{(T_1 - T_2)^2}{T_1 T_2} \geq 0$$

Total entropy is non-decreasing; irreversibility.

Port-Hamiltonian framework is not general enough !

Next:

to formulate a geometric theory of thermodynamic systems, generalizing the port-Hamiltonian formulation of multi-physics systems.

1. From Gibbs' relation to contact geometry
2. From contact geometry to homogeneous symplectic geometry
3. Definition of port-thermodynamic systems

Outline

Consider a simple thermodynamic system:

extensive variables V, S, E

intensive variables $-P, T$

Its state properties are formalized by Gibbs' relation

$$dE = TdS - PdV$$

(*More generally; in case of chemical reactions*:

extensive variables, $V, N_1, \cdots, N_m, S, E$

intensive variables $-P, \mu_1, \cdots, \mu_m, T$

Gibbs' relation extends to

$$dE = TdS - PdV + \mu_1 dN_1 + \cdots + \mu_m dN_m \ )$$

What does Gibbs' relation $dE = TdS - PdV$ mean?

Answer: If E is expressed as function of the other extensive variables V, S

$$E = E(V, S),$$

then the two intensive variables $-P, T$ are determined as

$$-P = \frac{\partial E}{\partial V}(V, S), \quad T = \frac{\partial E}{\partial S}(V, S)$$

Another quote:

Every mathematician knows that it is impossible to understand any elementary course in thermodynamics.
The reason is that the thermodynamics is based,
- as Gibbs has explicitly proclaimed -,
on a rather complicated mathematical theory,
on the contact geometry.

Vladimir I. Arnold,
Contact geometry: the geometrical method of Gibbs's thermodynamics,

(Proc. of the Gibbs Symposium, American Mathematical Society, 1989)

Basic contact geometry

Consider on the space $\mathbb{R}^5 \ni (V, S, E, -P, T)$ of extensive and intensive variables the contact form

$$\theta := dE - TdS + PdV,$$

State properties are given by maximal submanifolds $L \subset \mathbb{R}^5$ restricted to which θ is zero; i.e., on L

$$0 = dE - TdS + PdV \qquad \text{Gibbs' relation}$$

Any such L is 2-dimensional.

L is called a Legendre submanifold of $(\mathbb{R}^5, \theta)$.

Outline

Since the 1970's contact geometry has been recognized as appropriate geometric framework for thermodynamics.

On the other hand, contact geometry does not intrinsically distinguish between extensive and intensive variables, and state properties may also be written in entropy representation

$$S = S(V, E),$$

together with accompanying relations

$$\frac{1}{T} = \frac{\partial S}{\partial E}(V, E), \quad \frac{P}{T} = \frac{\partial S}{\partial V}(V, E)$$

This results from rewriting Gibbs' relation as

$$dS = \frac{1}{T} dE + \frac{P}{T} dV,$$

leading to different intensive variables $\frac{1}{T}$, $\frac{P}{T}$, and different contact form

$$\tilde{\theta} = dS - \frac{1}{T} dE - \frac{P}{T} dV$$

From contact to homogeneous symplectic geometry (Balian & Valentin, 2001)

Multiply the contact form

$$\theta = dE - TdS + PdV$$

on $\mathbb{R}^5$ by an extra variable p_E to obtain the Liouville form

$$\alpha := p_E dE + p_S dS + p_V dV, \quad p_S := -p_E T,\ p_V := p_E P$$

on the cotangent bundle $T^*\mathbb{R}^3 = \mathbb{R}^6$.

Energy representation corresponds to intensive variables

$$\frac{p_S}{-p_E} =: T, \quad \frac{p_V}{-p_E} =: -P$$

Entropy representation corresponds to intensive variables

$$\frac{p_E}{-p_S} = \frac{1}{T}, \quad \frac{p_V}{-p_S} = \frac{P}{T}$$

Thus: (p_V, p_S, p_E) *are homogeneous coordinates for intensive variables.*

General geometric picture

Start with $(n+1)$-dimensional manifold Q^e of extensive variables: $q^e = (E, S, V, \cdots)$.

Coordinates for the cotangent space $T^*_{q^e} Q^e$ are homogeneous coordinates for the intensive variables $T, -P, \cdots$.

Define the contact manifold $\mathbb{P}(T^*Q^e)$ as the projectivization of T^*Q^e: the $(2n+1)$-dimensional fiber bundle over Q^e with fiber at any point $q^e \in Q^e$ given by the n-dimensional projective space $\mathbb{P}(T^*_{q^e} Q^e)$.

This unifies energy and entropy representations, and is crucial for definition of power and entropy flow ports !

Furthermore, objects on odd-dimensional $\mathbb{P}(T^*Q^e)$ translate into easier homogeneous objects on even-dimensional T^*Q^e !

Objects on $\mathbb{P}(T^*Q^e)$ from homogeneous objects on T^*Q^e

Homogeneity of functions:

Definition

$K : T^*Q^e \to \mathbb{R}$ is homogeneous of degree r in p^e if

$$K(q^e, \lambda p^e) = \lambda^r K(q^e, p^e), \quad \forall \lambda \neq 0$$

Theorem (Euler)

$K : T^*Q^e \to \mathbb{R}$ is homogeneous of degree r iff

$$\sum p_i^e \frac{\partial K}{\partial p_i^e}(q^e, p^e) = r\, K(q^e, p^e), \qquad \text{for all } (q^e, p^e) \in T^*Q$$

Furthermore, if K is homogeneous of degree r (in p^e), then derivatives $\frac{\partial K}{\partial p_i^e}$ are homogeneous of degree $r - 1$.

Correspondence Legendre submanifolds $L \subset \mathbb{P}(T^*Q^e)$ and homogeneous Lagrangian submanifolds $\mathcal{L} \subset T^*Q^e$

T^*Q^e is endowed with Liouville form

$$\alpha = p_E dE + p_S dS + p dq, \quad q^e = (E, S, q) \quad (\text{e.g., } q = V, \cdots)$$

and the symplectic form

$$\omega = d\alpha = dp_E \wedge dE + dp_S \wedge dS + dp \wedge dq, \quad p^e = (p_E, p_S, p)$$

A Lagrangian submanifold is a maximal submanifold $\mathcal{L} \subset T^*Q$ restricted to which ω is zero.

Lagrangian $\mathcal{L} \subset T^*Q$ is homogeneous if

$$(q^e, p^e) \in \mathcal{L} \Rightarrow (q^e, \lambda p^e) \in \mathcal{L}$$

for any $0 \neq \lambda \in \mathbb{R}$.

Consider the canonical projection

$$\pi : T^*Q^e \to \mathbb{P}(T^*Q^e)$$

Then: any Legendre submanifold $L \subset \mathbb{P}(T^*Q^e)$ defines a homogeneous Lagrangian submanifold

$$\mathcal{L} := \pi^{-1}L \subset T^*Q^e,$$

and conversely any homogeneous Lagrangian submanifold is of this type. Furthermore:

Theorem

Homogeneous Lagrangian submanifolds $\mathcal{L} \subset T^*Q^e$ are maximal submanifolds restricted to which the Liouville one-form α is zero.

(Hence, not only $\omega := d\alpha$ is zero on $\mathcal{L}$, but in fact α is zero on $\mathcal{L}$!)

Outline

State space: a paradigm shift

Gibbs' relation describes state properties; i.e., relation between extensive and intensive variables.

Thus Legendre submanifold $L \subset \mathbb{P}(T^*Q^e)$ and homogeneous Lagrangian submanifold $\mathcal{L} \subset T^*Q^e$ describe the actual state space of the thermodynamic system !

Situation may be compared with description of capacitor: its 'state properties' are

$$E = E(q) \quad (= \frac{1}{2}q^2), \quad V = \frac{dE}{dq}(q) \quad (= \frac{q}{C})$$

This defines the 1-dimensional Legendre submanifold

$$L = \{E, q, V) \mid E = E(q),\ V = \frac{dE}{dq}(q)\}$$

describing the state space.
Corresponding 2-dim. homogeneous Lagrangian submanifold $\mathcal{L} \subset \mathbb{R}^4$.

Dynamics leaving L and $\mathcal{L}$ invariant

Recall that given $K : T^*Q^e \to \mathbb{R}$ the Hamiltonian vector field X_K on T^*Q^e with coordinates (q^e, p^e) is

$$\dot{q}^e = \frac{\partial K}{\partial p^e}(q^e, p^e), \quad \dot{p}^e = -\frac{\partial K}{\partial q^e}(q^e, p^e)$$

Any Hamiltonian vector field X_K is characterized by property $\mathbb{L}_{X_K}\omega = 0$.

X_K on T^*Q with K homogeneous (of degree 1 in p^e) not only satisfies $\mathbb{L}_{X_K}\omega = 0$, but in fact

$$\mathbb{L}_{X_K}\alpha = i_X d\alpha + d(\alpha(X_K)) = -dK + dK = 0$$

Conversely, if $\mathbb{L}_X\alpha = 0$, then $X = X_K$ with $K = \alpha(X)$ homogeneneous.

Furthermore, any Hamiltonian vector field X_K with K homogeneous of degree 1 projects to contact vector field $X_{\widehat{K}}$ on contact manifold $\mathbb{P}(T^*Q)$.

Summary: correspondence between *contact* and *homogeneous symplectic* geometry and dynamics

- Contact manifold $\mathbb{P}(T^*Q^e) \leftrightarrow$ symplectized manifold T^*Q^e
- Locally defined contact form θ on $\mathbb{P}(T^*Q^e) \leftrightarrow$ Liouville form α on T^*Q^e
- Functions on $\mathbb{P}(T^*Q^e) \leftrightarrow$ functions on T^*Q^e that are homogeneous of degree 0 in p^e
- Legendre submanifold $L \leftrightarrow$ homogeneous Lagrangian submanifold $\mathcal{L}$
- Generating function for $L \leftrightarrow$ homogeneous generating function for $\mathcal{L}$
- Contact Hamiltonian $\widehat{K} \leftrightarrow$ homogeneous Hamiltonian K
- Contact vector field $X_{\widehat{K}} \leftrightarrow$ Hamiltonian vector field X_K with $\mathbb{L}_{X_K}\alpha = 0$
- Invariance of L: $\widehat{K}$ zero on $L \leftrightarrow$ invariance of $\mathcal{L}$: K zero on $\mathcal{L}$

Definition of port-thermodynamic system

State properties are given by homogeneous $\mathcal{L} \subset T^*Q^e$.

Dynamics are given by homogeneous Hamiltonian, parametrized by $u \in \mathbb{R}^m$

$$K := K^a + K^c u : T^*Q^e \to \mathbb{R}, \quad u \in \mathbb{R}^m,$$

with K^a (drift Hamiltonian) and $K^c_j, j = 1, \cdots, m$ (input Hamiltonians), which are all zero restricted to $\mathcal{L}$.

By Euler's Theorem, homogeneity implies

$$K^a = p_E f_E + p_S f_S + p^T f, \quad f_E = \frac{\partial K^a}{\partial p_E}, f_S = \frac{\partial K^a}{\partial p_S}, f = \frac{\partial K^a}{\partial p}$$
$$K^c = p_E g_E + p_S g_S + p^T g, \quad g_E = \frac{\partial K^c}{\partial p_E}, g_S = \frac{\partial K^c}{\partial p_S}, g = \frac{\partial K^c}{\partial p}$$

where the functions f_E, f_S, f, g_E, g_S, g are all homogeneous of degree 0;

defining the dynamics of the extensive variables.

Additional conditions on the drift part K^a

First Law of Thermodynamics ('conservation of energy') imposes

$$f_E|_{\mathcal{L}} = 0$$

Second Law of Thermodynamics ('increase of entropy') imposes

$$f_S|_{\mathcal{L}} \geq 0$$

Interaction with environment through ports

Define the outputs (homogeneous degree 0)

$$y_p := g_E|_{\mathcal{L}},$$

leading to the power balance $\frac{d}{dt}E|_{\mathcal{L}} = y_p u$.

(u, y_p) defines a power port.

Entropy-conjugate outputs (again homogeneous degree 0) are defined as

$$y_e := g_S|_{\mathcal{L}},$$

leading to the entropy flow balance $\frac{d}{dt}S|_{\mathcal{L}} \geq y_e u$.

(u, y_e) defines a entropy flow port.

Example (Mass-spring-damper system)

Consider extensive variables z (extension of the spring), π (momentum) and entropy S. State properties are described by Lagrangian submanifold $\mathcal{L}$ with generating function

$$-p_E\left(\frac{1}{2}kz^2+\frac{\pi^2}{2m}+U(S)\right),$$

defining the state properties

$$\begin{aligned}\mathcal{L} \;=\; & \{(z,\pi,S,E,p_z,p_\pi,p_S,p_E)\mid E=\tfrac{1}{2}kz^2+\tfrac{\pi^2}{2m}+U(S),\\ & p_z=-p_E kz, p_\pi=-p_E\tfrac{\pi}{m}, p_S=-p_E U'(S)\}\end{aligned}$$

Dynamics is given by the homogeneous Hamiltonian

$$K=p_z\frac{\pi}{m}+p_\pi\left(-kz-d\frac{\pi}{m}\right)+p_S\frac{d(\frac{\pi}{m})^2}{U'(S)}+\left(p_\pi+p_E\frac{\pi}{m}\right)u$$

The power-conjugate output $y_p=\frac{\pi}{m}$ is the velocity of the mass.

Example (Gas-piston-damper system)

This system is analogous to previous example, replacing z by volume V and the partial energy $\frac{1}{2}kz^2 + U(S)$ by internal energy of the gas $U(V, S)$.

Dynamics is defined by the Hamiltonian

$$K = p_z \frac{\pi}{m} + p_\pi \left(-\frac{\partial U}{\partial V} - d\frac{\pi}{m} \right) + p_S \frac{d(\frac{\pi}{m})^2}{\frac{\partial U}{\partial S}} + \left(p_\pi + p_E \frac{\pi}{m} \right) u,$$

where the power-conjugate output $y_p = \frac{\pi}{m}$ is the velocity of the piston.

Thank you !

Questions?

Some key references for power networks

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