2017-02-14

DENSITY EVOLUTION {UNCERTAINTY PROPAGATION}

Consider $\dot{x} = f(x)$. Let $\Phi_t^f : \mathbb{R}^n \to \mathbb{R}^n$ denote associated flow map, i.e.

$\Phi_t^f(x_0)$ = solution to the differential equation $\dot{x} = f(x)$ evaluated at time t, with initial condition $x(t')|_{t'=0} = x_0$.

Here without further elaboration we assume that the given ODE satisfies conditions for existence and uniqueness, so that for (open) domain $D \subset \mathbb{R}^n$,

$$\Phi_t^f : D \to \mathbb{R}^n$$

is smooth and has smooth inverse on $\Phi_t^f(D)$.

Recall that if Y is an m-dimensional random variable $= \Psi(X)$ = image under a smooth and smoothly invertible transformation $\Psi : \mathbb{R}^m \to \mathbb{R}^m$ of another m-dimensional random variable X, with density $p_X(x)$, then Y has density

(1) $$p_Y(y) = p_X(\Psi^{-1}(y)) \Big/ \left|\det\left(\frac{\partial \Psi}{\partial x}\right)\right|_{x=\Psi^{-1}(y)}$$

(this is the "change of variables formula").

Suppose the initial condition for $\dot{x} = f(x)$ is random with density $p_0(x)$. Using the change of variables formula above we

seek to determine how the density evolves.
Clearly

(2) $$\rho\left(t, \Phi_t^f(x)\right) \cdot \det\left(\frac{\partial \Phi_t^f}{\partial x}\right) = \rho_0(x)$$

Differentiate both sides to obtain

$$0 = \frac{d}{dt}\left(\rho\left(t, \Phi_t^f(x)\right) \cdot \det\left(\frac{\partial \Phi_t^f}{\partial x}\right)\right)$$

$$= \left(\frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \frac{\partial \rho}{\partial x_i} \cdot \frac{d}{dt}\left(\Phi_t^f(x)^i\right)\right) \cdot \det\left(\frac{\partial \Phi_t^f}{\partial x}\right)$$

(CHAIN RULE)

$$+ \rho \cdot \frac{d}{dt}\left(\frac{\partial \Phi_t^f}{\partial x}\right)$$

$$= \left(\frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \frac{\partial \rho}{\partial x_i} f^i\left(\Phi_t^f(x)\right)\right) \cdot \det\left(\frac{\partial \Phi_t^f}{\partial x}\right)$$

(3) $$+ \rho \frac{d}{dt}\left(\det\left(\frac{\partial \Phi_t^f}{\partial x}\right)\right)$$

(DEFINITION of FLOW)

$$= (\mathrm{I}) + (\mathrm{II})$$

In (I), $\rho = \rho\left(t, \Phi_t^f(x)\right)$ and the arguments for partial derivatives are as for ρ.

To evaluate (II), let us denote

$$g(t) \triangleq \frac{\partial \Phi_t^f}{\partial x}$$

(suppressing the dependence on x to avoid clutter).

(4) $$\det(g) = \sum_{j=1}^{n} g_{ij} C_{ij}$$

for any $i \in \{1, 2, \dots, n\}$. Here C_{ij} denotes the cofactor of the $(i,j)^{th}$ element of the matrix g, i.e. $(-1)^{i+j}$. the determinant of the $(n-1) \times (n-1)$ submatrix of g obtained by removing the i^{th} row and j^{th} column. Clearly C_{ij} does <u>not</u> include the variable g_{ij}.

By chain rule,

$$\frac{d}{dt}\det(g) = \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial}{\partial g_{ij}}\det(g) \; \frac{d g_{ij}}{dt}$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} C_{ij} \frac{d}{dt} g_{ij} \qquad \text{from (4)}$$

$$= tr\left(C^T \dot{g}\right)$$

where $C^T = [C_{ij}]^T$ = transpose of matrix of cofactors

On the other hand $g^{-1} = \dfrac{C^T}{\det(g)}$,

equivalently $\quad C^T = \det(g)\, g^{-1}$

Thus

$$\frac{d}{dt}\det(g) = \operatorname{tr}\left(\det(g)\, g^{-1}\dot{g}\right)$$

$$= \det(g)\cdot \operatorname{tr}\left(g^{-1}\dot{g}\right)$$

$$= \det(g)\cdot \operatorname{tr}\left(\dot{g}\, g^{-1}\right)$$

We compute,

$$\dot{g} = \frac{d}{dt}\frac{\partial \Phi^f_t}{\partial x} = \left[\frac{d}{dt}\frac{\partial {\Phi^f_t}^{i}}{\partial x_j}\right]$$

$$= \left[\frac{\partial}{\partial x_j}\frac{d}{dt}{\Phi^f_t}^{i}\right]$$

$$= \left[\frac{\partial}{\partial x_j} f^i\left(\Phi^f_t(x)\right)\right]$$

$$= \left[\frac{\partial f^i}{\partial x_k}\left(\Phi^f_t(x)\right)\cdot \frac{\partial {\Phi^f_t}^{k}}{\partial x_j}\right]$$

(CHAIN RULE)

$$= \frac{\partial f}{\partial x}\left(\Phi^f_t(x)\right)\ \frac{\partial \Phi^f_t}{\partial x}$$

(5)

$$= \frac{\partial f}{\partial x}\left(\Phi^f_t(x)\right)\ g$$

Thus

$$\frac{d}{dt}\det(g) = \det(g)\ \mathrm{tr}\left(\dot{g}\, g^{-1}\right)$$

$$= \det(g)\ \mathrm{tr}\left(\frac{\partial f(\Phi_t^f(x))}{\partial x}\right)$$

(6) $$= \det\left(\frac{\partial \Phi_t^f(x)}{\partial x}\right) \sum_{i=1}^{n} \frac{\partial f^i}{\partial x_i}(\Phi_t^f(x))$$

It follows that

$$0 = (\mathrm{I}) + (\mathrm{II})$$

$$= \det\left(\frac{\partial \Phi_t^f(x)}{\partial x}\right) \cdot \left\{ \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n}\left(\frac{\partial \rho}{\partial x_i} f^i + \rho \frac{\partial f^i}{\partial x_i}\right)\right\}$$

Since $\det\left(\frac{\partial \Phi_t^f(x)}{\partial x}\right) \neq 0$ (recall Φ_t^f is invertible), it follows that

$$0 = \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \frac{\partial (\rho f^i)}{\partial x_i}$$

(7) $$= \frac{\partial \rho}{\partial t} + \mathrm{div}(\rho f) \qquad \blacksquare$$

This is Liouville's theorem.

suppose $n = 2K$, $x = (q_1, q_2, \dots, q_K, p_1, p_2, \dots p_K)$,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \qquad i = 1, 2, \dots, K.$$

Then

$$f = \begin{pmatrix} \frac{\partial H}{\partial p} \\ -\frac{\partial H}{\partial q} \end{pmatrix} \qquad \text{(Hamiltonian vector field)}$$

Then

$$\operatorname{div}(f) = \sum_{i=1}^{2K} \frac{\partial f^i}{\partial x_i} = \sum_{i=1}^{K} \left(\frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} \right)$$

$$= 0$$

Hence

$$0 = \frac{\partial \rho}{\partial t}(t, q, p) + \operatorname{div}(\rho f)$$

$$= \frac{\partial \rho}{\partial t}(t, q, p) + \sum_{i=1}^{K} \left(\frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right)$$

$$= \frac{d\rho}{dt} \Big|$$ along trajectories of $\dot{x} = f(x)$, hamiltonian vector field

= convective derivative

This is a conservation law (GIBBS)

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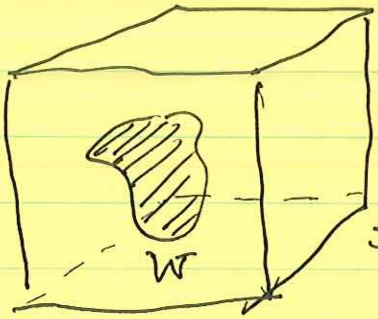
FLUIDS VIEW

of Liouville's Theorem



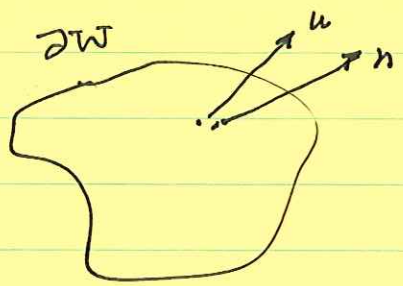
W fixed subregion of D, does not change with time.

$$\frac{d}{dt} m(W, t) = \frac{d}{dt} \int_W \rho(x, t)\, dV$$

$$= \int_W \frac{\partial}{\partial t} \rho(x, t)\, dV$$

W smooth, ∂W smooth

n outward normal unit vector



dA area element on ∂W

volume flow rate across ∂W per unit area $= u \cdot n$

mass flow rate $= \rho\, u \cdot n$

Rate of increase of mass in W
= rate at which mass is crossing the boundary ∂W inward direction

$$\frac{d}{dt} \int_W \rho\, dV = - \int_{\partial W} \rho\, u \cdot n\, dA$$

2 $\Rightarrow \dfrac{d}{dt} \displaystyle\int_{W} \rho \, dV = - \int_{W} \operatorname{div}(\rho u) \, dV$

by divergence theorem.

$$\Rightarrow \int_W \left(\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) \right) dV = 0$$

Holds for all W

$$\Rightarrow \quad \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho u) = 0$$