Moment Closure - A Brief Review

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Motivation

Consider a general evolution equation:

$$\partial_t u = F(u), \qquad u = u(t) \in \mathcal{X}.$$

Could be a ODE, PDE, IDE, DDE, SODE, network, etc.

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- dimension reduction (if $\dim(\mathcal{X}) = \infty$ or $\dim(\mathcal{X}) \gg 1$)
- many methods "work well in practice"
- only few methods have been proven to be accurate

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MOMENT CLOSURE falls into this scheme

Moment Closure - Three Concrete Examples

(I) **Stochastic differential equations**

- Kolmogorov equation ($\dim(\mathcal{X}) = \infty$)
- moments $\leftrightarrow$ moments of a probability density

(II) **Kinetic theory**

- Boltzmann-type mesoscopic models ($\dim(\mathcal{X}) = \infty$)
- moments $\leftrightarrow$ certain integrals

(III) **Network dynamics**

- dynamics of graph, nodes, edges ($\dim(\mathcal{X}) \gg 1$)
- moments $\leftrightarrow$ graph motives

(I) Stochastic Ordinary Differential Equations (SODEs)

Standard SODE ($x \in \mathbb{R}$ for simplicity) on $(\Omega, \mathcal{F}, \mathbb{P})$

$$x' = f(x) + \sigma\xi, \qquad ' = \frac{\mathrm{d}}{\mathrm{d}t}.$$

$\xi = W'$ (W = Brownian motion), $\sigma > 0$

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$$f(x) := a_2 x^2 + a_1 x + a_0.$$

- x depends upon the random input space $\Rightarrow$ random variable
- define expectation/mean/averaging $\mathbb{E}[\cdot] := \langle \cdot \rangle$
- might want to know **moments**: $m_j := \langle x^j \rangle$

Calculating moment equations...

Just average:

$$m_1{}' = \langle x' \rangle = a_2 \langle x^2 \rangle + a_1 \langle x \rangle + a_0 = a_2 m_2 + a_1 m_1 + a_0 .$$

$\Rightarrow$ Need second moment equation!

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Using Itô's formula one finds

$$(x^2)' = [2xf(x) + \sigma^2] \; + 2x\sigma \; \xi' .$$

Just average:

$$\begin{aligned} m_2' &= 2\langle a_2 x^3 + a_1 x^2 + a_0 x \rangle + \sigma^2 + \sigma \langle 2x\xi \rangle \\ &= 2(a_2 m_3 + a_1 m_2 + a_0 m_1) + \sigma^2 , \end{aligned}$$

(where $\langle 2x\xi \rangle = 0$ as $\int_0^t 2x(s) \, \mathrm{d}W_s$ is a martingale)

Main Steps

First steps:

(S0) **moment space:** select the space $\mathbb{M} = \{m_j\}$.

(S1) **moment equations:** derive evolution equations for m_j.

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- system in (S1) is frequently infinite
- infinite system not a desirable reduction
- nonlinearity is crucial
- hierarchical structure

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Next steps:

(S2) **moment closure:** "higher moments from lower moments"

(S3) **verfication:** does the closed system approximate dynamics?

Kolmogorov Equation / Fokker-Planck Equation

Probability density $p = p(x, t|x_0, t_0)$ of x at time t

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}[(a_2 x^2 + a_1 x + a_0)p] + \frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2}.$$

Step (S1) to derive the moment equation:

- note: $m_j = \int_{\mathbb{R}} x^j \; p(x,t) \,\mathrm{d}x$
- multiply Fokker-Planck by x^j and average

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For example, we have

$$\begin{aligned} {m_1}' &= \langle x' \rangle = \int_{\mathbb{R}} x \frac{\partial p}{\partial t}\, \mathrm{d}x \\ &= \int_{\mathbb{R}} -x \frac{\partial}{\partial x}[(a_2 x^2 + a_1 x + a_0)p]\, \mathrm{d}x + \int_{\mathbb{R}} x \frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2}\, \mathrm{d}x. \end{aligned}$$

If p and its derivatives vanish at infinity then

$${m_1}' = \int_{\mathbb{R}} [(a_2 x^2 + a_1 x + a_0)p]\, \mathrm{d}x = a_2 m_2 + a_1 m_1 + a_0$$

(II) Kinetic Equations

Basics:

- spatial variable $x \in \Omega \subset \mathbb{R}^N$
- momentum variable $v \in \mathbb{R}^N$
- gas via a single-particle density $\varrho = \varrho(x, v, t)$

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Kinetic equation (mesoscopic dynamics)

$$\frac{\partial \varrho}{\partial t} + v \cdot \nabla_x \varrho = Q(\varrho),$$

where

- $\nabla_x = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_N})^\top$
- suitable boundary conditions are assumed
- $\varrho \mapsto Q(\varrho)$ is the collision operator

Moment Equations for Kinetic Equation

Instead of probabilistic average, take velocity average

$$\langle G \rangle := \int_{\mathbb{R}^N} G(x, v, t)\, \mathrm{d}v$$

Same (similar) procedure:

- pick polynomial space $\mathbb{M}$ with $\{m_j = m_j(v)\}$
- multiply the kinetic equation by basis elements
- average, using velocity averaging
- get (infinite!) hierarchy of moment equations

Remark: classical closure is Grad's 13 moment system (in 1949)

(III) Network Dynamics - SIS Model

Basics:

- goal: model epidemics on a network/graph
- graph with nodes in states S and I
- SI-link: infection at rate τ
- I-node: recovery at rate γ
- $m_I := \langle I \rangle = \langle I \rangle(t)$ average number of infected
- $m_S = \langle S \rangle = \langle S \rangle(t)$ average number of susceptibles

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Formal (statistical physics) derivation yields

$$\begin{aligned} \frac{\mathrm{d}m_S}{\mathrm{d}t} &= \gamma m_I - \tau \langle SI \rangle, \\ \frac{\mathrm{d}m_I}{\mathrm{d}t} &= \tau \langle SI \rangle - m_I, \end{aligned}$$

where $\langle SI \rangle =: m_{SI}$ = average number of SI-links.

Second-order equations (Keeling; Rand; Taylor et al.):

$$\begin{aligned}
\frac{\mathrm{d}m_{SI}}{\mathrm{d}t} &= \gamma(m_{II} - m_{SI}) + \tau(m_{SSI} - m_{ISI} - m_{SI}),\\
\frac{\mathrm{d}m_{II}}{\mathrm{d}t} &= -2\gamma m_{II} + 2\tau(m_{ISI} + m_{SI}),\\
\frac{\mathrm{d}m_{SS}}{\mathrm{d}t} &= 2\gamma m_{SI} - 2\tau m_{SSI}.
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Observations:

- different derivation strategies
- typical **moment closure** problem
- number of equations grows rapidly

Abstract Moment Closure Problem

Infinite-dimensional moment system

$$
\begin{aligned}
\frac{\mathrm{d}m_1}{\mathrm{d}t} &= h_1(m_1, m_2, \ldots), \\
\frac{\mathrm{d}m_2}{\mathrm{d}t} &= h_2(m_2, m_3, \ldots), \\
\frac{\mathrm{d}m_3}{\mathrm{d}t} &= \cdots,
\end{aligned} \tag{1}
$$

Moment closure: "high-order moments via lower-order moments"

$$H(m_1, \ldots, m_\kappa) = (m_{\kappa+1}, m_{\kappa+2}, \ldots).$$

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Final result:

$$\begin{aligned} \frac{\mathrm{d}m_1}{\mathrm{d}t} &= h_1(m_1, m_2, \ldots, m_\kappa, H(m_1, \ldots, m_\kappa)), \\ \frac{\mathrm{d}m_2}{\mathrm{d}t} &= h_2(m_1, m_2, \ldots, m_\kappa, H(m_1, \ldots, m_\kappa)), \\ \vdots &= \vdots \\ \frac{\mathrm{d}m_\kappa}{\mathrm{d}t} &= h_\kappa(m_1, m_2, \ldots, m_\kappa, H(m_1, \ldots, m_\kappa)). \end{aligned} \tag{2}$$

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(Q1) How to find/select the mapping H?

(Q2) How well does (2) approximate (1)?

Some Classical Closures

(I) Probability theory closures, e.g., consider SODE case

$$
\begin{aligned}
m_j &= 0 \quad \text{if } j \geq 3 \text{ and } j \text{ is odd,} \\
m_j &= (m_2)^{j/2}\,(j-1)(j-3)\cdots 2 \quad \text{if } j \geq 4 \text{ and } j \text{ is even.}
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(II) Physical principle closures, e.g., consider kinetic case

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\min_{\varrho}\{\langle \varrho \ln \varrho - \varrho\rangle : \langle M\varrho\rangle = \eta\} = H(\eta),
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de-correlation closure!

Lots of (applied) mathematics work...

Stochastic systems:

- SODEs: Arnold, Bobryk, Bolotin, Grigoriu, Nasell, Singer, ...
- Discrete models: Baake, Gower, Leslie, ...

Kinetic equations:

- max-ent & theory: Devilettes, Grad, Levermore, Torrilhon, ...
- applications: Christen, Kassubek, Klar, Struchtrup, ...

Networks:

- stat-phys: Gleeson, Gross, Kirkwood, Kiss, Shaw, Schwartz, ...
- epidemiology: Dieckmann, Eames, House, Keeling, ...
- ecology: Bolker, Pacala, Matis, Rand, Volz, ...

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$\rightarrow$ "Moment closure - a brief review", **CK**, arXiv:1505.02190

Conjecture(s) / Direction(s)

- Closures work only on restricted assumptions.
- Dynamical systems view has to be (re-)introduced.
- Proofs will need algebraic and analytical tools.

Motivation: Fast-Slow Systems

Fast variables $x \in \mathbb{R}^m$, slow variables $y \in \mathbb{R}^n$, time scale separation $0 < \varepsilon \ll 1$.

$$\left\{\begin{array}{rcr} x' & = & f(x,y) \\ y' & = & \varepsilon g(x,y) \end{array}\right. \quad \overset{\varepsilon t = s}{\longleftrightarrow} \quad \left\{\begin{array}{rcl} \varepsilon \dot{x} & = & f(x,y) \\ \dot{y} & = & g(x,y) \end{array}\right.$$

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fast subsystem / slow subsystem

- Think: $x =$ higher-order moments, $y =$ lower-order moments!

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fast subsystem slow subsystem

- Think: $x =$ higher-order moments, $y =$ lower-order moments!

- $C_0 := \{f = 0\} =$ critical manifold $=$ equil. of fast subsystem.
- C_0 is normally hyperbolic if $\mathrm{D}_x f$ has no zero-real-part eigenvalues.
- **Fenichel's Thm:** Normal hyperbolicity $\Rightarrow$ "nice" perturbation C_ε.

The Last Slide...

Summary & Outlook:

- many open problems...
- combinatorial: How many equations? Structures?
- algebraic: Symmetries/invariants? Normal forms?
- probabilistic: Stochastic closures? Microscopic closures?
- analytical: Error estimates? Entropy closure validity?
- geometric: Slow manifolds? Geometry of moment space?
- dynamical: Capturing bifurcations? Phase-space dissection?

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Papers, preprints, etc all available from:

- **www.asc.tuwien.ac.at/∼ckuehn** and **arXiv**

- "Moment closure - a brief review", Christian Kuehn, arXiv:1505.02190
- "Multiple Time Scale Dynamics", Christian Kuehn, Springer, 2015

Thank you very much for your attention!