Modeling uncertainties with kinetic equations

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Section 1

Motivations
Need in applied sciences

- Assume the probability law is given
  
  \[ d\mathcal{P} = d\mu(\omega), \quad d\mathcal{P} = e^{-\frac{(\omega-\omega_0)^2}{2\sigma}} d\omega, \quad \omega \in \mathbb{R}^P \text{ high stochastic dimension.} \]

- A popular idea to use chaos polynomials (Wiener 36’) expansion

  \[ u(x, t, \omega) \approx u_N(x, t, \omega) = \sum_{0}^{N} u_n(x, t)p_n(\omega), \quad p_n \in P_n. \]
Goal: model/propagate uncertainties in conservation laws

- **Euler equations** (Wiener 38', Lin-Su-Karniadakis 06', Glimm and al 06', …)

\[
\begin{aligned}
\partial_t \rho + \partial_x (\rho v) &= 0, \\
\partial_t (\rho v) + \partial_x (\rho v^2 + p_\omega) &= 0, \\
\partial_t (\rho e) + \partial_x (\rho ve + p_\omega v) &= 0,
\end{aligned}
\]

\[p_\omega = (\gamma(\omega) - 1)\rho \varepsilon\]

\[e = \varepsilon + \frac{1}{2} v^2.\]

- **Transport of the uncertain variable \(\omega\)**

\[
\begin{aligned}
\partial_t U + \partial_x F(U, \omega) &= 0, \\
\partial_t (\rho \omega) + \partial_x (\rho v \omega) &= 0.
\end{aligned}
\]

- In this presentation: model conservation law with uncertainties in the initial condition

\[
\begin{aligned}
\partial_t u + \partial_x F(u) &= 0, \\
u(x, \omega, 0) &= u_0(x, \omega)
\end{aligned}
\]

\[F : \mathbb{R} \to \mathbb{R},\]
Section 2

Kinetic formulations
Kinetic formulation of conservation laws

- The kinetic formulation of conservation laws (Perthame-Tadmor 91') writes

\[
\begin{align*}
\partial_t f_\varepsilon + a(\xi) \partial_x f_\varepsilon + \frac{1}{\varepsilon} f_\varepsilon = \frac{1}{\varepsilon} M(u_\varepsilon; \xi), & \quad a(\xi) = F'(\xi), \quad \text{(Burgers : } a(\xi) = \xi), \\
u_\varepsilon(x, t) = \int f_\varepsilon(x, \xi, t) d\xi, & \\
f_\varepsilon(t = 0) = M(u^{\text{init}}; \xi),
\end{align*}
\]

For simplicity \(u^{\text{init}} \geq 0\). The kinetic variable is \(\xi \geq 0\). The pseudo-Maxwellian is \(M(u; \xi) = \mathbf{1}_{\{0 < \xi < u\}}\).

- Under general conditions (Lions-Perthame-Tadmor 94'), the limit \(\varepsilon \to 0^+\) is:

\[
u_\varepsilon(t) \to u(t) \text{ in } L^1_x \text{ and } f_\varepsilon(t) \to M(u(t)) \text{ in } L^1_{x\xi}
\]

\[
\partial_t u + \partial_x F(u) = 0, \quad F : \mathbb{R} \to \mathbb{R}.
\]

Moreover the limit is entropic (we will come back to that).
Variables:

usual variables are the time $t$ and space $x$, additionally one has the kinetic variable $\xi$ and the uncertain variable $\omega$.

Consider

\[
\begin{cases}
\partial_t f^N_{\epsilon} + a(\xi) \partial_x f^N_{\epsilon} + \frac{1}{\epsilon} f^N_{\epsilon} = \frac{1}{\epsilon} M^N (u^N_{\epsilon}; \xi, \omega), \\
u^N_{\epsilon}(x, \omega, t) = \int f^N_{\epsilon}(x, \xi, \omega, t) d\xi, \\
f^N_{\epsilon}(t = 0) = M^N (u^{\text{init}}; \xi, \omega),
\end{cases}
\]

where $0 \leq M^N (u^N_{\epsilon}; \xi, \omega) \leq 1$ is a suitable polynomial approximation of $M$.

Strategy: construct $M^N$, study properties and pass to the limit $\epsilon \to 0$ and $N \to \infty$. 
Convolutions with polynomial kernels

Convolution

\[ M^N(u^N_\epsilon; \xi) = G^N \ast_{\omega} M(u^N_\epsilon; \xi) = \int G^N(\omega, \omega') M(u^N_\epsilon(\omega'); \xi) d\mu(\omega') \in P^N_{\omega} \]

with kernel \( G^N(\omega, \omega') = \sum_{n=0}^{N} c_n p_n(\omega) p_n(\omega') \), with \( p_n \) the orthonormal basis of polynomials for the measure \( d\mu(\omega) \) and where \( c_n \) are appropriate coefficients, and where \( G^N \) is a Kernel Polynomial Method (Weisse and al, 2006)

\[ G^N \geq 0, \quad \int G^N(\omega, \omega') d\mu(\omega') = 1. \tag{1} \]

Basic example: Take \( d\mu(\omega) = \frac{d\omega}{\pi \sqrt{1 - \omega^2}} \), on \( \omega \in I = (-1, 1) \), and Tchebycheff orthonormal polynomials \( p_n(\omega) = T_n(\omega) = \cos(n \arccos \omega), -1 \leq \omega \leq 1 \). The Fejer kernel \( G^N_F \) is defined by the coefficients

\[ c_0 = 1 \text{ and } c_n = 2 \frac{N + 1 - n}{N + 1}, \quad 1 \leq n \leq N \]

\[ f^N_F(\omega) = c_0 \mu_0 + 2 \sum_{n=1}^{N} c_n \mu_n T_n(\omega), \quad \mu_n = \int_I f(\omega') T_n(\omega') d\mu(\omega') \]

\[ f^N_F(\cos t) = \int_0^{2\pi} f(\cos u) K^N_F(t - u) du, \quad K^N_F(u) = \frac{1}{2\pi(N + 1)} \left( \frac{\sin(N + 1)\frac{u}{2}}{\sin\frac{u}{2}} \right)^2 \geq 0. \]
A priori estimates

\[
\begin{align*}
\partial_t f^N_{\epsilon} + a(\xi) \cdot \nabla f^N_{\epsilon} + \frac{1}{\epsilon} f^N_{\epsilon} &= \frac{1}{\epsilon} G^N \ast \omega \ M(u^N_{\epsilon}; \xi, \omega), \\
\quad u^N_{\epsilon}(x, \omega, t) &= \int f^N_{\epsilon}(x, \xi, \omega, t) d\xi.
\end{align*}
\]

- $L^\infty$ bounds: $0 \leq f^N_{\epsilon} \leq 1$, $0 \leq u^N_{\epsilon} \leq U_M := \sup_{x, \omega} u^{\text{init}}(x, \omega)$,
  \[f^N_{\epsilon}(x, \xi, \omega, t) \equiv 0 \text{ for } \xi \geq U_M.\]

- Entropy bounds $S''(\xi) \geq 0$:
  \[
  \partial_t \int S'(\xi) f^N_{\epsilon}(x, \xi, \omega, t) d\xi d\mu(\omega) + \text{div} \int a(\xi) S'(\xi) f^N_{\epsilon}(x, \xi, \omega, t) d\xi d\mu(\omega) \leq 0
  \]

- Propagation of classical BV bounds:
  \[
  \begin{align*}
  \int |\nabla_x f^N_{\epsilon}| dx d\xi d\mu(\omega) &\leq C^{\text{init}}, \\
  \int |\nabla_x u^N_{\epsilon}| dx d\mu(\omega) &\leq C^{\text{init}}, \\
  \int |\partial_t f^N_{\epsilon}(t)| dx d\xi d\mu(\omega) &\leq \int |\partial_t f^N_{\epsilon}(0)| dx d\xi d\mu(\omega) \leq C^{\text{init}}, \\
  \int |\partial_\xi f^N_{\epsilon}(t)| dx d\xi d\mu(\omega) &\leq e^{-\frac{t}{\epsilon}} \int |\partial_\xi f^N_{\epsilon}(0)| dx d\xi d\mu(\omega) + C
  \end{align*}
  \]

- Plus new BV estimates with respect to $\omega$, using the convolution structure.
Convergence for all $t \geq 0$ (Jackson kernels)

- **The limit is a weak solution** $N^2 \varepsilon \to \infty$ : Consider the Jackson kernels. There exists $f \in L^1_{loc}(D_0)$ such that $\lim_{\varepsilon \to 0} \left\| f^N_\varepsilon - f \right\|_{L^1_{loc}(D_0)} = 0$ and

$$\partial_t f + a(\xi) \partial_x f = \partial_\xi m$$
weak solution

where $m \geq 0$ is a measure, and $f = M(u; \xi)$ with $u = \int f d\xi$.

"So" (Lions-Perthame-Tadmor 94') : $u$ is the solution (a.e.).

- **Strong error bounds** $N \varepsilon \to \infty$ : Moreover

$$\left\| f^N_\varepsilon(t) - G^N *_\omega f_\varepsilon(t) \right\|_{L^1_{x,\xi,\mu}} \leq C \frac{t}{\varepsilon} \int_0^{2\pi} |f(\cos(t + \alpha) - f(\cos t)| dt \approx \frac{Ct}{N \varepsilon}.$$

- **Projected equations** $\varepsilon = \frac{1}{N+1}$ fixed : One gets for

$$u^N_{\varepsilon,i}(x, t) = \int f^N_{\varepsilon,i}(x, \xi, \omega, t) d\xi d\mu(\omega), \quad f^N_{\varepsilon,i}(x, \omega, t) = \int f^N_{\varepsilon}(x, \xi, \omega, t) T_i(\omega) d\xi$$

$$\partial_t u^N_{\varepsilon,i} + \partial_x \int a(\xi) f^N_{\varepsilon,i} d\xi = -h_N(i)u^N_{\varepsilon,i}, \quad h_N(i) > 0 \text{ for } i > 0.$$
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Section 3

Kinetic polynomials and optimal control
• Reminder Brenier 83': the indicatrix function is the minimum of a certain minimization problem

\[ 1_{\{0 < \xi < u\}} = M(u; \cdot) = \arg\min_{\{0 \leq g \leq 1\| \int g d\xi = u \geq 0\}} \int_0^\infty g(\xi)S'(\xi)d\xi, \quad \forall S, \ S'' > 0. \]

• Generalize: Minimization of weighted \( L^1 \) norms, under convex constraints

\[ M^N(u^N) = \arg\min_{g^N \in K^N(u^N)} \int_0^\infty \int_I g^N(\xi, \omega)S'(\xi)d\xi d\mu(\omega), \quad \text{for admissible } S, \]

where

\[ K^N(u^N) = \left\{ g^N(\cdot, \cdot) \in P^N_\omega, \ u^N(\omega) = \int_0^\infty g^N(\xi, \omega)d\xi, \ 0 \leq g^N \leq 1 \text{ for } \omega \in I \right\} \]
A remark

Make the assumption: for all $u^N \geq 0$ there exists a unique $M^N$ (we call it a kinetic polynomial) such that

$$M^N(u^N) = \underset{g^N \in K^N(u^N)}{\text{argmin}} \int_0^\infty \int_I g^N(\xi, \omega) S'(\xi) d\xi d\mu(\omega), \quad \text{for a given } S.$$

Then the solution of

$$\begin{cases}
    \partial_t f^N_\varepsilon + a(\xi) \partial_x f^N_\varepsilon + \frac{1}{\varepsilon} f^N_\varepsilon = \frac{1}{\varepsilon} M^N(u^N_\varepsilon; \xi, \omega), \\
    u^N_\varepsilon(x, \omega, t) = \int f^N_\varepsilon(x, \xi, \omega, t) d\xi, \\
    f^N_\varepsilon(t = 0) = M^N(u^{\text{init}}; \xi, \omega),
\end{cases}$$

is in bounds, $0 \leq f^N \leq 1$, and is conservative

$$\partial_t u^N_\varepsilon(x, \omega, t) + \partial_x G^N_\varepsilon(x, \omega, t) d\xi = 0,$$

$$u^N_\varepsilon = \int_{\xi} f^N_\varepsilon d\xi, \quad G^N_\varepsilon(x, \omega, t) = \int_{\xi} a(\xi) f^N_\varepsilon d\xi.$$

This last property does not hold with the convolution method.
Moreover it satisfies the entropy inequality
\[
\frac{d}{dt} \int_{\xi} \int_{\omega} \int_{x} f^N(x, \xi, \omega, t) dx S'(\xi) d\xi d\mu(\omega)
\]
\[
= \frac{1}{\varepsilon} \int_{x} \left( \int_{\xi} \int_{\omega} M^N S'(\xi) d\xi d\omega - \int_{\xi} \int_{\omega} f^N S'(\xi) d\xi d\omega \right) \leq 0.
\]
Note that it passes (at least formally) to the limit $\varepsilon \to 0$ : one gets the equation
\[
\partial_t u^N(x, \omega, t) + \partial_x G^N(x, \omega, t) d\xi = 0, \quad G^N(x, \omega, t) = \int_{\xi} a(\xi) M^N(u^N) d\xi
\]
which satisfies the entropy inequality
\[
\partial_t \int_{\xi} a(\xi) M^N(u^N) d\xi + \partial_x \int_{\xi} a(\xi) M^N(u^N) S'(\xi) d\xi \leq 0.
\]
Designing $M^N$ is the issue

For simplicity rewrite the time and space variables as $t \leftarrow \xi$ and $x \leftarrow \omega$. Set $S'(\xi) = S'(t) = t$ for simplicity. Consider the interval $x \in I = [0, 1]$. write $n = N$. The problem rewrites as :

Given a given non negative polynomial $u_n \in P_n^+(I)$, find

$$v_n(t) \in U_n \equiv \{w_n \in P_n \mid 0 \leq w_n(x) \leq 1 \text{ for all } x \in I\}$$

with the constraint

$$\int_0^T v_n(t, x) dt = u_n(x) \quad x \in I,$$

such that

$$v_n = \arg\min \int_0^T \int_I w_n(t, x) t dt dx.$$

the structure of $U_n$ is complex with an infinite number of constraints and the functional is linearly degenerate.

:) it can interpreted in the setting of Optimal Control.
Set

\[ y_n(t, x) = \int_0^T v_n(t, x) dt. \]

The problem writes: Find a control \( v_n(t) \in U_n \) such that the state \( y_n \)

\[ \frac{d}{dt} y_n = v_n, \quad y_n(0) = 0, \]

reaches the objective \( y_n(T) = u_n \) and minimizes the cost function

\[ C(v_n) = \int_0^T \int_I v_n(t, x) t dtdx. \]

**First obvious result:** if \( T \geq \|u_n\|_{L^\infty} \) then

\[ v_n^{\text{non opt.}}(t, x) = \frac{u_n(x)}{\|u_n\|_{L^\infty}} \]

is a (a priori) non optimal solution.
Properties

- Wish/claim: there exists a unique solution $v_n(t)$ to the Optimal control problem. Hint of the proof: mix the Bojanic-Devore theorem (one-sided $L^1$ polynomial approximation) with optimal control.

- **Theorem** (Pontryagin maximum principle): for all optimal trajectories, there exists a multiplier $\lambda_n \in P_n$ such that
  - either the trajectory is normal
    $$v_n(t) = \arg\max_{w_n \in U_n} \int_0^1 (\lambda_n(x) - t)w_n(x)\,dx$$
  - or the trajectory is abnormal
    $$v_n(t) = \arg\max_{w_n \in U_n} \int_0^1 \lambda_n(x)w_n(x)\,dx.$$ 

- Next simulations are with the AMPL code, very popular in the Optimal Control community.
Feasible solution: constant one layer the other

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Feasible solution: constant one layer the other

\[ \xi_{L+1} = 0 \]
\[ \xi_1 = u_+ \]
\[ \xi_0 = 0 \]

M=1
second layer
last non zero layer
bottom layer
M=0
infinite upper layer
\[ \omega \]

Conclusion

Kinetic polynomials/DFG-CNRS Workshop 2016
Numerical scheme (with the feasible solution)

Let a 1D mesh $j \Delta x$. Consider

$$\frac{\bar{u}^N_j - u^N_j}{\Delta t} + \frac{F^N[u^N_j] - F^N[u^N_{j-1}]}{\Delta x} = 0,$$

unknown $u^N_j \in P^N(\omega)$ is a polynomial in $\omega$ of degree $N$ (fixed) in cell $j$, flux $F^N[u^N_j] \in P^N(\omega)$ in cell $j$ is constructed with the kinetic polynomial formula for the Burgers equation

$$F^N[u^N]_n = \sum_{l \geq 0} (F(\xi_{l+1}) - F(\xi_l)) \int h^N_l(\omega)p_n(\omega)d\mu(\omega), \quad F(\xi) = \frac{\xi^2}{2}.$$

Assume init. is bounded: $0 \leq U_m \leq u^N_j(\omega) \leq U_M < \infty$, $\forall j$ and $\forall \omega \in I$.

**Theorem**: Assume the CFL condition $U_M \Delta t \leq \Delta x$. Then

$$U_m \leq \bar{u}^N_j(\omega) \leq U_M, \quad \forall j \text{ and } \forall \omega \in I.$$

Proof. Either use the kinetic formulation, or prove directly.
Numerical illustration: Burgers equation

Set up: \( d\mu(\omega) = \frac{d}{\pi \sqrt{1-\omega^2}} \), \( N = 2 \).

The moments model is explicit

\[
\partial_t \begin{pmatrix} a \\ b \\ c \end{pmatrix} + \partial_x \begin{pmatrix} \frac{a^2+b^2+c^2}{2} \\ ab + \frac{bc}{\sqrt{2}} \\ ac + \frac{b^2}{2\sqrt{2}} \end{pmatrix} = 0.
\]

Compare solutions of
- the moment model,
- the kinetic polynomial method with feasible solution,
- and the standard non intrusive approach (quadrature points, close to MC).
Consider the system of $N + 1$ conservation laws with $d\mu(\omega) = d\omega$

$$
\begin{cases}
\partial_t u_0 + \partial_x \int_{-1}^{1} \left( \sum_{n \leq N} u_n \varphi_n(\omega) \right)^2 \varphi_0(\omega) d\omega = 0, \\
\vdots \\
\partial_t u_n + \partial_x \int_{-1}^{1} \left( \sum_{n \leq N} u_n \varphi_n(\omega) \right)^2 \varphi_N(\omega) d\omega = 0.
\end{cases}
$$

- There is an entropy-entropy flux pair $\implies$ hyperbolicity

$$
\partial_t \sum_{n \leq N} |u_n|^2 + \partial_x \int_{\Theta} \left( \sum_{n \leq N} u_n \varphi_n(\omega) \right)^3 d\omega \leq 0.
$$
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Shock

\[ u^{\text{ini}}(x, \omega) = \begin{cases} 
3 & \text{for } x < 1/2 \text{ and } -1 < \omega < 0, \\
5 & \text{for } x < 1/2 \text{ and } 0 < \omega < 1, \\
1 & \text{for } 1/2 < x \text{ and } -1 < \omega < 1.
\end{cases} \]

projection of the initial data

exact solution \( t = 0.4 \)

moment solution \( t = 0.4 \)

new method \( t = 0.4 \)
Compressive solution

\[ u^{ini}(x, \omega) = \begin{cases} 
12 & \text{for } x - \omega/5 < 1/2, \\
1 & \text{for } x - \omega/5 < 3/2, \\
12 - 11(x - \omega/5 - 1/2) & \text{in between.}
\end{cases} \]
Non intrusive moments with quadrature points

Use $\omega_1 = -\sqrt{\frac{3}{4}}$, $\omega_2 = 0$ and $\omega_3 = \sqrt{\frac{3}{4}}$. Then reconstruct.

reconstructed initial data           reconstructed solution at $t = 0.1$

The test is performed with the compressive initial data.

Initialization of the shock problem is ambiguous at $t = 0$. 
Larger $N$ (with a moment method, Poette PHD)
Conclusion

- The kinetic formulation of conservation laws is a convenient tool for the analysis of conservation laws with intrusive uncertainties.
- The theory of convolution-based method is OK, but the practice not clear due the spurious damping.
- The alternative is kinetic polynomials (Maxwellian plus polynomials) which are at their infancy.
  The theory is full of open problems: existence, uniqueness, error estimates, ... and connection with optimal control.

Two issues were not addressed in this talk:
interpretation of the results in terms of probability; the curse of dimension \( \omega \in \mathbb{R}^{\text{large}} \).