Algorithmic issues for the modeling of uncertainties in kinetic equations

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Introduction
A mathematical approach to the propagation of uncertainties (variable $\omega$) in conservation laws

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

\[
\begin{aligned}
\partial_t \rho + \partial_x (\rho v) &= 0, \\
\partial_t (\rho v) + \partial_x (\rho v^2 + p_\omega) &= 0, \\
\partial_t (\rho e) + \partial_x (\rho ve + p_\omega v) &= 0, \\
p_\omega &= (\gamma(\omega) - 1)\rho\varepsilon \\
e &= \varepsilon + \frac{1}{2}v^2.
\end{aligned}
\]

- **Transport of the uncertain variable $\omega$**

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

- **Non linear model conservation law with uncertainties in the initial condition**

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

For simplicity of the exposure, $u_0 \geq 0$ and $F'(u) \geq 0$. 

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Kinetic formulation (Perthame-Tadmor 91’)

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

For simplicity \( u^{\text{init}} \geq 0 \). The pseudo-Maxwellian is \( M(u; \xi) = 1_{\{0 < \xi < u\}} \).
• We note the minimization principle for convex entropies $S$

\[ \int_0^\infty M(u; \xi)S'(\xi)d\xi \leq \int_0^\infty f_\varepsilon(\xi)S'(\xi)d\xi \]

and

\[ \int_0^\infty M(u, \xi)d\xi = \int_0^\infty f_\varepsilon(\xi)d\xi = u. \]

from which the basic entropy-like inequality is deduced

\[ \partial_t \int_0^\infty \varepsilon(x, \xi, t)S'(\xi)d\xi + \partial_x \int_0^\infty a(\xi)f_\varepsilon(x, \xi, t)S'(\xi)d\xi \leq 0. \]

• Under general conditions (Lions-Perthame-Tadmor 94'), the limit $\varepsilon \to 0^+$ is: $u_\varepsilon(t) \to u(t)$ in $L^1_x$ and $f_\varepsilon(t) \to M(u(t))$ in $L^1_{x,\xi}$

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

- Variables are now \((t, x, \xi, \omega)\). Consider

\[
\begin{align*}
\partial_t f_\varepsilon^n + a(\xi) \partial_x f_\varepsilon^n + \frac{1}{\varepsilon} f_\varepsilon^n &= \frac{1}{\varepsilon} M_n(u_\varepsilon^n; \xi, \omega), \\
u_\varepsilon^n(x, \omega, t) &= \int f_\varepsilon^n(x, \xi, \omega, t) d\xi, \\
f_\varepsilon^n(t = 0) &= M_n(u^{\text{init}}_\varepsilon; \xi, \omega),
\end{align*}
\]

where \(M_n(u_\varepsilon^n; \xi, \omega)\) is a suitable polynomial approximation of \(M\).

- Suitable means \(M_n(u, \xi, \cdot) \in U_n\) with

\[
U_n = \{ p_n(y) \in P_n, \ 0 \leq p_n(y) \leq 1 \text{ for } 0 \leq y \leq 1 \}.
\]

- Strategy:
  construct \(M_n\),
  study properties,
  pass to the limit \(\varepsilon \to 0\) and \(n \to \infty\),
  get more information on \(U_n\).

D.-Perthame, Uncertainty propagation; intrusive kinetic formulations of scalar conservation laws, JUQ.
Section 2

Method I
Convolutions with polynomial kernels

**Convolution**

\[ M_n(u^n_\varepsilon; \xi) = G^n * \omega M(u^n_\varepsilon; \xi) = \int G^n(\omega, \omega') M(u^n_\varepsilon(\omega'); \xi) d\mu(\omega') \in U_n \]

with kernel \( G^n(\omega, \omega') = \sum_{r=0}^{n} c_r p_r(\omega) p_r(\omega') \), with \( p_r \) the orthonormal basis of polynomials for the measure \( d\mu(\omega) \) and where \( c_r \) 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

\( c_0 = 1 \) and \( c_r = \frac{n+1-r}{n+1}, \quad 1 \leq r \leq n \)

\[ f^n_F(\omega) = c_0 \mu_0 + 2 \sum_{r=1}^{n} c_r \mu_r T_r(\omega), \quad \mu_r = \int I f(\omega') T_r(\omega') d\mu(\omega') \]

\[ f^n_F(\cos t) = \int_{0}^{2\pi} f(\cos u) K^n_F(t-u) du, \quad K^n_F(u) = \frac{1}{2\pi (n+1)} \left( \frac{\sin(n+1)u}{\sin \frac{u}{2}} \right)^2 \geq 0. \]
Convergence for all $t \geq 0$ (Jackson kernels)

• **Strong error bounds** $n\varepsilon \to \infty$ : Consider the Jackson kernels (better approximation than Fejer kernel)

\[
\| f^n_\varepsilon (t) - G^n \ast_\omega f_\varepsilon (t) \|_{L^1_{x\xi\mu}} \leq C \frac{t}{\varepsilon} \int_0^{2\pi} |f(\cos(t + \alpha)) - f(\cos t)| \, dt \approx \frac{Ct}{n\varepsilon}.
\]

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

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

\[
 \partial_t u^n_{\varepsilon,i} + \partial_x \int a(\xi) f^n_{\varepsilon,i} \, d\xi = -h_n(i) u^n_{\varepsilon,i}, \quad h_n(i) > 0 \text{ for } i > 0.
\]

• There is **spurious damping** of the moments $i > 0$.

• The issue is the definition of $M_n$. 

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Section 3

Method II
Kinetic polynomials

- Reminder: the indicatrix function is the optimum of the minimization problem Brenier 83'

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

Design principle of kinetic polynomials:
Minimization of weighted \( L^1 \) norms, under convex constraints:

\[ M_n(u^n) = \arg\min_{g^n \in K^n(u^n)} \int_0^\infty \int_I g^n(\xi, \omega) S'(\xi) d\xi d\mu(\omega), \]

where

\[ K^n(u^n) = \left\{ g^n(\cdot, \cdot) \in U_n(\cdot), \int_0^\infty g^n(\xi, \omega) d\xi = u^n(\omega) \right\}. \]

- For \( n = 0 \), this is the usual criterion.
Uniqueness of kinetic polynomials

• Claim 1 (th.) (D.-Trelat) : for a given $S$, there exists (easy part) a unique (difficult part) solution $M_n$

$$M_n(u^n) = \arg\min_{g^n \in K^n(u^n)} \int_0^\infty \int_I g^n(\xi, \omega) S'(\xi) d\xi d\mu(\omega).$$

- Therefore the solution of

$$\begin{cases}
\partial_t f_\varepsilon^n + a(\xi)\partial_x f_\varepsilon^n + \frac{1}{\varepsilon} f_\varepsilon^n = \frac{1}{\varepsilon} M_n(u^n_\varepsilon; \xi, \omega), \\
u^n_\varepsilon(x, \omega, t) = \int f^n_\varepsilon(x, \xi, \omega, t)d\xi, \\
f_\varepsilon^n(t = 0) = M_n(u^{\text{init}}_\varepsilon; \xi, \omega),
\end{cases}$$

is in bounds ($0 \leq f^n \leq 1$), is conservative (much better than convolution)

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

$$u^n_\varepsilon = \int_\xi f^n_\varepsilon d\xi, \quad G^n_\varepsilon(x, \omega, t) = \int_\xi a(\xi)f^n_\varepsilon d\xi$$

and has the entropy property

$$\partial_t \int_0^\infty f_\varepsilon^n S'(\xi)d\xi + \partial_x \int_0^\infty a(\xi)f^n_\varepsilon S'(\xi)d\xi \leq 0, \quad \forall t, x, \omega.$$
Reformulation as optimal control

For simplicity only, take $S'(s) = s$ and decide of a given $\xi > 0$. Note $v_n = M_n$ with

$$y_n(\xi, \omega) = \int_0^\xi v_n(s, \omega) ds.$$ 

The problem for $M_n$ writes:

Find a control $v_n(s) \in U_n$ such that the state $y_n$

$$\frac{d}{ds} y_n = v_n, \quad y_n(0) = 0,$$

reaches the objective

$$y_n(\xi, \omega) = u_n(\omega)$$

and minimizes the cost function

$$C(v_n) = \int_0^\xi \int_I v_n(s, \omega) s ds d\omega.$$
• **Theorem 2** (Pontryagin maximum principle, D.-Trelat, preprint soon available) : for all optimal trajectories, there exists a multiplier $\lambda_n \in P_n$ such that

  - either the trajectory is normal

    $$v_n(s) = \arg\max_{w_n \in U_n} \int_0^1 (\lambda_n(\omega) - s) w_n(\omega) d\omega$$

  - or the trajectory is abnormal

    $$v_n(s) = \arg\max_{w_n \in U_n} \int_0^1 \lambda_n(\omega) w_n(\omega) d\omega.$$
• All trajectories are normal.

• For almost all $s$, $M_n(s, \cdot) = v_n^{\text{opt}} \in U_n$ has points of contact at 0 and 1

$$M_n(s, \omega_i) = 0$$

for $i = 0, 1, \ldots$

The order of the contact is $\geq n + 1$.

• Next simulation are with the AMPL code (thanks E. Trélat), very popular in the Optimal Control community. This is constraint optimization.

Example of the code follows:

```AMPL
var u {k in 0..n, i in 0..Nt};
var utx {i in 0..Nt-1, j in 0..Nx} = sum{k in 0..n} u[k,i]*(j/Nx)^k;
subject to cont{i in 0..Nt-1, j in 0..Nx}:
0 <= utx[i,j] <= 1;
```
Section 4

Method III
- $U_n$ is everywhere in scientific computing
- High order approximation of functions with low regularity is always polluted with oscillations

On the Suppression of Numerical Oscillations . . .
Shyy and al (JCP 92’)

- We spent years to control oscillations \textbf{a posteriori} for non linear equations: shock waves, contact discontinuities, . . ., limiters, . . .
Starting point

To get standard polynomial notations: \( x \leftarrow \omega \).

**Lukacs theorem:** Two cases occur.

- Either \( n = 2m \in 2\mathbb{N} \), then there exists \( a_m \in P_m \) and \( b_{m-1} \in P_{m-1} \) such that
  \[
  p_n = a_m^2 + b_{m-1}^2 \omega \quad w(x) = x(1-x). \tag{2}
  \]

- Or \( n + 1 = 2m \in 2\mathbb{N} \), then there exists \( a_{m-1} \in P_m \) and \( b_{m-1} \in P_{m-1} \) such that
  \[
  p_n = a_{m-1}^2 w_1 + b_{m-1}^2 w_2 \quad w_1(x) = x, \quad w_2(x) = 1 - x. \tag{3}
  \]

- It could be used to model high order approximations of positive functions (think of \( \rho, T, \ldots \)).

Classical textbooks on polynomials are
- Szego : Orthogonal polynomials, 39’.
- Milovanovic and al : Topics in polynomials : extremal problems, inequalities, zeros, 82’.
- Devore-Lorenz : Constructive approximation, 81’.
Two bounds

• Start with $p \in U_n$.

• $p \in P_n^+$: the Lukacs theorem yields the representation

$$p = a^2w_1 + b^2w_2$$  \hspace{1cm} (4)

where $a$ and $b$ are polynomials with convenient degree and $w_1$ and $w_2$ are the weights.

• $1 - p \in P_n^+$: so

$$1 - p = c^2w_3 + d^2w_4$$ \hspace{1cm} (5)

where $c$ and $d$ are polynomials with convenient degree. The weights $w_3$ and $w_4$ are a priori equal to $w_1$ and $w_2$.

• That is

$$1 = a^2w_1 + b^2w_2 + c^2w_3 + d^2w_4.$$  \hspace{1cm} (6)
4-squares Euler identity

It writes

\[
\hat{A}^2 + \hat{B}^2 + \hat{C}^2 + \hat{D}^2 = \left( \hat{a}^2 + \hat{b}^2 + \hat{c}^2 + \hat{d}^2 \right) \left( \hat{\alpha}^2 + \hat{\beta}^2 + \hat{\gamma}^2 + \hat{\delta}^2 \right) \tag{7}
\]

where

\[
\begin{align*}
\hat{A} &= \hat{a}\hat{\alpha} + \hat{b}\hat{\beta} + \hat{c}\hat{\gamma} + \hat{d}\hat{\delta} \\
\hat{B} &= \hat{a}\hat{\beta} - \hat{b}\hat{\alpha} + \hat{c}\hat{\delta} - \hat{d}\hat{\gamma} \\
\hat{C} &= \hat{a}\hat{\gamma} - \hat{b}\hat{\delta} - \hat{c}\hat{\alpha} + \hat{d}\hat{\beta} \\
\hat{D} &= \hat{a}\hat{\delta} + \hat{b}\hat{\gamma} - \hat{c}\hat{\beta} - \hat{d}\hat{\alpha}.
\end{align*}
\tag{8}
\]

- Itard : les nombres premiers, PUF, 69'.
Introduce the weights by setting

\[\hat{a} = \sqrt{w_1} a, \quad \hat{b} = \sqrt{w_2} b, \quad \hat{c} = \sqrt{w_3} c, \quad \hat{d} = \sqrt{w_4} d,\]  
(9)

\[\hat{\alpha} = \sqrt{w_1} \alpha, \quad \hat{\beta} = \sqrt{w_2} \beta, \quad \hat{\gamma} = \sqrt{w_3} \gamma, \quad \hat{\delta} = \sqrt{w_4} \delta,\]  
(10)

and

\[\hat{A} = \sqrt{w_1} A, \quad \hat{B} = \sqrt{w_2} B, \quad \hat{C} = \sqrt{w_3} C, \quad \hat{D} = \sqrt{w_4} D.\]  
(11)

Start from \((a, b, c, d)\) and \((\alpha, \beta, \gamma, \delta)\) which satisfy (6) : it yields

\[
\begin{align*}
A &= \sqrt{w_1} a\alpha + \sqrt{\frac{w_2}{w_1}} b\beta + \sqrt{\frac{w_3}{w_1}} c\gamma + \sqrt{\frac{w_4}{w_1}} d\delta, \\
B &= \sqrt{w_1} a\beta - \sqrt{w_1} b\alpha + \sqrt{\frac{w_3 w_4}{w_2}} c\delta - \sqrt{\frac{w_3 w_4}{w_2}} d\gamma, \\
C &= \sqrt{w_1} a\gamma - \sqrt{\frac{w_2 w_4}{w_3}} b\delta - \sqrt{w_1} c\alpha + \sqrt{\frac{w_2 w_4}{w_3}} d\beta, \\
D &= \sqrt{w_1} a\delta + \sqrt{\frac{w_2 w_3}{w_4}} b\gamma - \sqrt{\frac{w_2 w_3}{w_4}} c\beta - \sqrt{w_1} d\alpha.
\end{align*}
\]  
(12)
Matrix of the weight

- It can be rewritten as

\[
\begin{pmatrix}
A \\
B \\
C \\
D
\end{pmatrix} = M
\begin{pmatrix}
a \\
b \\
c \\
d
\end{pmatrix}
\]

where \( M \) is a \( 4 \times 4 \) matrix.

- The issue is that \((A, B, C, D)\) are not necessarily polynomials, since the square root of fractions of polynomial weights show up.

- To investigate the constraints brought by the weights, we simplify \( M \) by keeping only the weights. One obtains the \( 4 \times 4 \) matrix of the weights

\[
W = \begin{pmatrix}
\sqrt{w_1} & \sqrt{\frac{w_2}{w_1}} & \sqrt{\frac{w_3}{w_1}} & \sqrt{\frac{w_4}{w_1}} \\
\sqrt{w_2} & \sqrt{w_1} & \sqrt{\frac{w_3 w_4}{w_2}} & \sqrt{\frac{w_3 w_4}{w_2}} \\
\sqrt{w_1} & \sqrt{\frac{w_2 w_3}{w_4}} & \sqrt{w_1} & \sqrt{\frac{w_2 w_4}{w_3}} \\
\sqrt{w_2} & \sqrt{\frac{w_2 w_3}{w_4}} b & \sqrt{\frac{w_2 w_3}{w_4}} & \sqrt{w_1}
\end{pmatrix}
\]
First solution: $w_1 = w_3 = 1$, 
$w_2 = w_4 = x - x^2 \equiv w$

\[
\begin{align*}
A &= a\alpha + wb\beta + c\gamma + wd\delta, \\
B &= a\beta - b\alpha + c\delta - d\gamma, \\
C &= a\gamma - wb\delta - c\alpha + wd\beta, \\
D &= a\delta + b\gamma - c\beta - d\alpha.
\end{align*}
\]  
(15)

• Set 
\[
\mathcal{U}_n = \{(a, b, c, d) \in P_n \times P_{n-1} \times P_n \times P_{n-1} \mid 1 = a^2 + b^2 w + c^2 + d^2 w\}
\]

such that $1 = a^2 + b^2 w + c^2 + d^2 w$.

• Assume $(a, b, c, d) \in \mathcal{U}_n$ and $(\alpha, \beta, \gamma, \delta) \in \mathcal{U}_m$. Then 
$(A, B, C, D) \in \mathcal{U}_{n+m}$. 
• The polynomials \((a, b, c, d) \in U_1\) can be written as

\[
\begin{align*}
    a(x) &= \cos \theta x + \cos \varphi (1 - x), \\
    b &= R \cos \mu, \\
    c(x) &= \sin \theta x + \sin \varphi (1 - x), \\
    d &= R \sin \mu,
\end{align*}
\]

where the angles \((\theta, \varphi, \mu) \in \mathbb{R}^3\) are arbitrary and \(R = 2 \sin \left( \frac{\theta - \varphi}{2} \right)\).

**Hint**: 

\[
\begin{align*}
    a(x)^2 + c(x)^2 + (b^2 + d^2)x(1 - x) \\
    = x^2 + (1 - x)^2 + \left( 2 \cos(\theta - \varphi) + R^2 \right) x(1 - x) \\
    = x^2 + (1 - x)^2 + 2x(1 - x) = 1
\end{align*}
\]

since \(\cos \tau = 1 - 2 \sin^2(\tau/2)\).

**Theor. 4 (D. Hal online)**: Any polynomial in \(U_n\) can be obtained with a repeated use of the formula (15) applied to at most \(n\) polynomials in \(U_1\).

**Corollary**: there exists a parametrization of \(U_{2n}\) with \(3n\) real coefficients.
Are the generating formulas efficient and stable?

- to answer this question, tests are performed within a Matlab test code with the `fminunc` function

- all problems considered below are written like

\[
\text{Find } p_n \in U_n \text{ such that } J(p_n) \leq J(q_n) \quad \forall q_n \in U_n
\]

where \( J \) is some functional. For example it can be the \( L^2 \) norm between \( p_n \) and a given objective function \( f \) : in this case
\[
J(q_n) = \left( \int_0^1 |f(x) - q_n(x)|^2 \, dx \right)^{\frac{1}{2}}.
\]

- the functional \( J(q_n) \) is in practice discretized as

\[
\mathcal{J}_h(\alpha) = \sum_i \omega_i J(q_n(x_i; \alpha)), \quad \alpha \in \mathbb{R}^{3n}.
\]

- \( \mathcal{J}_h \) may have local minima \( \alpha_1, \alpha_2, \ldots \) : we systematically run the calculation between 1 and 5 times and keep the best candidate.
The objective function which is the rescaled Tchebycheff polynomial

\[ f_2(x) = \frac{T_{20}(x) + 1}{2}. \]

We use 21 equi-distributed quadratures points. The calculation are performed with a polynomial degree \( p \in U_{10} \) and \( p \in U_{20} \).

On the left : minimization of a discrete \( L^2 \) norm between the rescaled Tchebycheff polynomial \( \frac{T_{20}(x) + 1}{2} \) and polynomials with bounds, \( n = 10, 20 \). The numerical solution is exact for \( n = 20 \).

On right : same problem with another loop for \( w_1 = x \) and \( w_2 = 1 - x \).
Consider the $L^2$ norm between $p(\alpha)$ and the Runge function properly rescaled in the bounds $[0, 1]$ as

$$f_1(x) = \frac{26}{25} \left( \frac{1}{1 + 25(2x - 1)^2} - \frac{2}{6} \right).$$

Three computations are performed with $n = 2, 4, 6$, $\alpha \in \mathbb{R}^{3n}$ and $p \in P_{2n}$. For each $n$ the functional $J_h$ is evaluated with $n + 1$ equi-distributed quadrature points. In terms of complexity it corresponds to Lagrange interpolation on a uniform grid.

The convergence in uniform norm is also proved by rigorous estimates.
Objective function is a step function

\[ f_4(x) = 0 \text{ for } x < 0.4 \text{ and } z(x) = 1 \text{ for } 0.4 < x. \]

The number of quadrature points is 25. The degree of the polynomials is 8, 16 and 24. The convergence in a discrete \( L^1 \) norm is observed. The respect of the bounds is perfect.
Checking kinetic polynomials

To check the PMP (Pontryagin Maximum Principle), maximize functionals like

\[ J(p_n) = \int_0^1 (\lambda_n(x) - t) p_n(x) \, dx, \quad p_n \in U_n \]  

(17)

where \( \lambda_n \in P_n \) is given and \( t \) may vary.

Take \( n = 3 \) and

\[ \lambda_2(x) = T_2(2x - 1) + x \]  

and \( t = 0.3 \).

A first numerical simulation yields the numerical value of the cost function is \( J(p_n^1) \approx 0.16737 \). The total order of contact if \( 1 + 2 + 2 = 5 \).
• The global minimum is captured by numerical simulations with another starting point. Now $J(p_n^2) \approx 0.188478 > J(p_n^1)$.

The total order of contact is equal to $2n + 1 = 7$ (since $n = 3$). It is now in accordance with the theory of kinetic polynomials.
2D : the main case

Take the weights $w_1 = 1$, $w_2 = 1 - x^2$, $w_3 = 1 - y^2$ $w_4 = w_2 w_3$ and the representation

$$p(x, y) = a(x, y)^2 w_1(x) + c(x, y)^2 w_2(x) + e(x, y)^2 w_3(y) + g(x, y)^2 w_4(x)$$

$$1 - p(x, y) = b(x, y)^2 w_1(x) + d(x, y)^2 w_2(x) + f(x, y)^2 w_3(y) + h(x, y)^2 w_4(x).$$

Note the redundancy due to $w_4$.

It yields a 8-squares formula

$$1 = \left( a(x, y)^2 + b(x, y)^2 \right) w_1(x) + \left( c(x, y)^2 + d(x, y)^2 \right) w_2(x)$$

$$+ \left( e(x, y)^2 + f(x, y)^2 \right) w_3(y) + \left( g(x, y)^2 + h(x, y)^2 \right) w_4(x).$$
Link with the 17th Hilbert theorem and Hurwiz theorem

• The 1-2-4-8 Hurwiz theorem yields an obstruction to many squares identity at any order. In particular no 6-squares identity available: this is the reason of the redundancy with $w_4$.

• For $n = 8$, the solution is given in the form of the Degen identity

$$(a^2 + b^2 + c^2 + d^2 + e^2 + f^2 + g^2 + h^2)(m^2 + n^2 + o^2 + p^2 + q^2 + r^2 + s^2 + t^2)$$

$$= (am-bn-co-dp-eq-fr-gs-ht)^2 + (bm+an+do-cp+fq-er-hs+gt)^2$$

$$+ (cm-dn+ao+bp+gq+hr-es-ft)^2 + (dm+cn-bo+ap+hq-gr+fs-et)^2$$

$$+ (em-fn-go-hp+aq+br+cs+dt)^2 + (fm+en-ho+gp-bq+ar-ds+ct)^2$$

$$+ (gm+hn+eo-fp-cq+dr+as-bt)^2 + (hm-gn+fo+ep-dq-cr+bs+at)^2.$$
Complex four squares identity

- It is convenient to rewrite it as an Euler identity with complex numbers. We define \((i^2 = -1)\)

\[ u = a + ib, \quad v = c + id, \quad w = e + if, \quad z = g + ih \quad (18) \]

and

\[ \alpha = m + in, \quad \beta = o + ip, \quad \gamma = q + ir, \quad \delta = s + it. \quad (19) \]

The Degen identity rewrites as

\[
|A|^2 + |B|^2 + |C|^2 + |D|^2 = \left( |u|^2 + |v|^2 + |w|^2 + |z|^2 \right) \left( |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 \right) \quad (20)
\]

with

\[
\begin{align*}
A &= u\alpha - v^*\beta - w\gamma^* - z^*\delta, \\
B &= v\alpha + u^*\beta + z\gamma^* - w^*\delta, \\
C &= w\alpha - z\beta^* + u^*\gamma + v^*\delta, \\
D &= z\alpha^* + w\beta - v\gamma + u\delta.
\end{align*}
\]
Elementary polynomials

- Elementary solutions with low degree are

  either \( \alpha = e^{i\theta} x + e^{i\varphi} (1 - x), \quad \beta = Re^{i\mu}, \quad \gamma = \delta = 0, \) (22)

  or \( \alpha = e^{i\theta} y + e^{i\varphi} (1 - y), \quad \gamma = Re^{i\mu}, \quad \beta = \delta = 0, \) (23)

  where the angles \( \theta, \varphi, \mu \in \mathbb{R} \) are arbitrary and \( R = 2 \sin \left( \frac{\theta - \varphi}{2} \right) \).

- The loop can be written as

\[
\begin{align*}
A &= u\alpha - v^*\beta w_2 - w\gamma^* w_3 - z^*\delta w_2 w_3, \\
B &= v\alpha + u^*\beta + z\gamma^* w_3 - w^*\delta w_3, \\
C &= w\alpha - z\beta^* w_2 + u^*\gamma + v^*\delta w_2, \\
D &= z\alpha^* + w\beta - v\gamma + u\delta
\end{align*}
\] (24)

where the weights are \( w_2(x) = 1 - x^2 \) and \( w_3(y) = 1 - y^2 \).
2D : smooth objective function

Cost function is the $L^2$ distance between $p_n$ and the objective function

$$f_5(x, y) = \frac{T_8((2x + y)/3) + 1}{2}.$$

One observes clear convergence when increasing $n$ (up to 16). For $n = 16$ the numerical value of the cost function is $\approx 0.0195$. 

11 × 11 quadrature points, $n = 4, 8, 16$ and $L^2$ norm.
Minimization of the discrete $L^2$ distance to the objective function

$$f_6(x, y) = H(2x + y), \quad H \text{ the Heaviside function.}$$

The $L^2$ distance is better in terms of the smoothness and speed of convergence. The number of quadrature points is $11 \times 11$ and $n = 10$ then 20.
Section 5

More numerical results
Numerical illustration: Burgers equation

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

\[
u(t, x, \omega) = a(t, x)u_0(\omega) + b(t, x)u_1(\omega) + c(t, x)u_2(\omega).
\]

The moments model is explicit

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

Compare solutions of

- the moment model,
- the kinetic polynomial method with feasible solution (projection of simplified kinetic polynomial),
- and the standard non intrusive approach (quadrature points, close to MC): not shown.
$u^{\text{ini}}(x, \omega) = \begin{cases} 
3 & \text{for } x < 1/2 \text{ and } -1 < \omega < 0, \\
5 & \text{for } x < 1/2 \text{ and } 0 < \omega < 1, \\
1 & \text{for } 1/2 < x \text{ and } -1 < \omega < 1. 
\end{cases}$
Compressive solution

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

This work is initially a mathematical approach for intrusive uncertainties.

- The kinetic formulation of conservation laws is a convenient tool.
- The theory is full of open problems: existence, uniqueness, error estimates, . . ., and connection with $L^1$ minimization techniques and optimal control.

It begins to be strongly complemented by robust and efficient algorithms.

- Algorithms coming from the optimal control community.
- The weighted 4-squares Euler identity (linked to quaternions algebras) yields an efficient parametrization of $U_n$.

The parametrization of $U_n$ is extremely appealing for many other applications in scientific computing.

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