DECAY RATES FOR KOLMOGOROV EQUATIONS AND ITS NUMERICAL APPROXIMATION SCHEMES.

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1. MOTIVATION

Build numerical schemes that preserve the long time behavior of PDEs.

Not always easy: Stability of numerical schemes often requires adding numerical viscosity that, often, increases artificially the decay of the numerical solutions as $t \to \infty$.

2. CONNECTIONS WITH STABILISATION

In the context of the stabilisation of control systems there are many examples where a suitable feedback ensures the exponential stabilisation as $t \to \infty$. See the huge literature on the stabilisation of wave equations.

But these properties are often lost under numerical discretisations: See SIAM Rev., 2005, paper by E.Z.

The same occurs with the dispersive properties of Schrödinger and KdV equations: See the works by L. Ignat and E.Z.

By the contrary, things are much easier for parabolic equations. They are so much dissipative that their nature is preserved under numerical discretisations.

What about hypoelliptic models like Kolmogorov equations?

3.- MAIN RESULT.

We shall see that for Kolmogorov equations the decay rate is preserved. But the analysis is much more subtle than for heat equations.

4.- PRELIMINARIES ON HEAT EQUATION

Consider the heat equation:

$$y_t - \Delta y = 0.$$

What about decay?

- In a bounded domain with Dirichlet boundary conditions the decay is exponential.

$$\|y(t)\|_{L^2} \leq e^{-\lambda_1 t} \|y_0\|_{L^2(\Omega)},$$

λ_1 being the first eigenvalue of the Dirichlet Laplacian.

The proof can be done by energy estimates using Poincaré inequality.

- In the full space the decay is polynomial but provided we assume further integrability conditions in the initial data.

For instance

$$\|y(t)\|_p \le C(p,d)\, t^{-\frac{d}{2}\left(1-\frac{1}{p}\right)} \|y_0\|_1 .$$

But note that the norm of the semigroup

$$S(t): L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$$

is $= 1$ and, therefore, the decay rate can be made arbitrarily slow for high frequency solutions.

The easiest proof of this decay is based on the representation by convolution with the Gaussian heat kernel and the use of Young's inequality:

$$G(x,t) = (4\pi t)^{-\frac{d}{2}} \exp\left(\frac{-|x|^2}{4t}\right).$$

But here we are interested on numerics:

- Do standard approximation schemes preserve these decay properties;
- Can these decay properties be obtained by the methods available at the PDE level?

The answer differs again from bounded to unbounded domains:

- For bounded domains energy methods work at the PDE level too;
- For unbounded domains and, in particular, in $\mathbb{R}^d$, the proof based on the use on the explicit heat kernel is not so straightforward.

But in $\mathbb{R}^d$ there are many different proof the polynomial decay. Here are some of them:

- Moser's iteration. Based on energy estimates using nonlinear powers of the solution as test functions, Holder inequality, Sobolev embedding, etc.
  It can be adapted to the discrete frame of numerical schemes.

- Similarity variables. Based mainly on the observation that the heat kernel has the scaling

$$G(x,t) = t^{-d/2} F(x/\sqrt{t}).$$

Then, roughly, one works on the new space variable $\overline{x} = \sqrt{t}\, x$.

This technique is not adapted to standard numerical schemes since it introducing a stretching of the space mesh, increasing as time increases!

• <u>Expansions of the initial data on the Dirac basis.</u>

For instance, it is easy to see that

$$y_0 = \int_{\mathbb{R}^d} y_0 \, dx \, \delta_0 + \operatorname{div}(\vec{Y_0})$$

with $\vec{Y_0} \in L^1(\mathbb{R}^d)$ whenever $y_0 \in L^1(\mathbb{R}^d; 1+|x|)$. Many variants of this result can be found in the CRAS Note by J. Duoandikoetxea & E.Z., 1992.

But these kinds of results are useful to make the asymptotic behavior more precise when the fundamental solution is available. Not of real use for discrete models.

• <u>Techniques based on improved energy or Lyapunov functionals.</u>

Classical for damped wave equations and developed for hypoelliptic models by Desvillettes, Villani, Hérau et al., under the name of hypocoercivity.

This is the point of view we shall successfully adopt for the numerical schemes of Kolmogorov!

5.- REMAINDER THE DAMPED WAVE EQUATION

There is an extensive literature on the stabilization of waves that uses this idea of hypocoercivity.

The most classical example is

$$y_{tt} - \Delta y + y_t = 0$$

on a bounded domain, with Dirichlet boundary conditions.

Then

$$E(t) = \frac{1}{2}\int_\Omega |\nabla y(x,t)|^2 + |y_t(x,t)|^2 dx$$

is such that

$$\frac{dE}{dt}(t) = -\int_\Omega |y_t|^2 dx.$$

This does not suffice for the exponential decay.

Then, one introduces

$$F_\varepsilon = E + \varepsilon \int_\Omega y y_t \, dx$$

such that

$$F_\varepsilon \sim E \quad \text{for } \varepsilon \text{ small}$$

and

$$\frac{dF_\varepsilon}{dt} \leq -c F_\varepsilon$$

which leads to the decay rate.

This construction is very much related to the classical Kalman rank condition of finite-dimensional control systems. This can be found in the paper by K. Beauchard & E.Z. on the decay of partially dissipative control systems.

Consider the finite-dimensional system

$$y' + Ay + BB^* y = 0 .$$

Then, if $A = -A^*$ by (A, B) satisfy the Kalman rank condition, it can be proved the solutions decay exponentially.

Note however that

$$\frac{d}{dt}\left[\frac{1}{2}|y(t)|^2\right] = -|B^* y(t)|^2 .$$

Thus the exponential decay is not obvious on this dissipation law.

One can build however other norms, based on the Kalman matrix, that we call Kalman norm

$$|x|^2 + \Sigma |B^* x|^2 + \cdots$$

Summarizing all these ideas we will build a robust method for the decay of numerical approximation schemes for Kolmogorov equations.

6.- DECAY FOR THE KOLMOGOROV EQUATION

$$f_t - f_{xx} - x f_y$$

A. Kolmogorov, Annals of Math., 1934.

This equation behaves very differently with respect to the classical convection-diffusion equation with constant convective term

$$f_t - f_{xx} - v f_y = 0.$$

In this case transport and diffusion do not interact:

$$f(x,y,t) = g(x, y+vt, t)$$

$$g(x,y,t) = f(x, y-vt, t)$$

Then

$$g_t - g_{xx} = 0 \iff f_t - f_{xx} - v f_y = 0.$$

Thus, there is regularizing effect in the x variable, but not on the y variable. Typical profiles would look like

$$(4\pi t)^{-\frac{1}{2}} \exp\left(-\frac{|x|^2}{4t}\right) \otimes \delta_{y+vt}(y)$$

Similarly, the decay is the one of the 1-d heat equation in the variable x. There is no other dissipative mechanism enhancing the decay.

But the solution of Kolmogorov's equation is Gaussian in all the variables:

$$K(x,y,t) = \frac{1}{3\pi^2 t^2} \exp\left[-\frac{1}{\pi^2}\left(3\frac{|y-(y_0+tx_0)|^2}{t^3} + 3\frac{|y-(y_0+tx_0))(x-x_0)}{t^2} + \frac{|x-x_0|^2}{t}\right)\right.$$

Surprisingly enough the fundamental equation of the kolmogorov equation decays like $1/t^2$, while the one of the convection-diffusion model with constant convection as $t^{-1/2}$ and the solution of the heat equation in dimension $d=2$ as t^{-1}!

Why kolmogorov equation decays faster?

Not because the energy dissipation law.

Both the kolmogorov and the convection-diffusion model show the same energy dissipation law:

$$\frac{1}{2}\frac{d}{dt}\iint f^2 \, dx dy = -\iint f_x^2 \, dx dy .$$

Furthermore, the heat equation looks even more dissipative:

$$\frac{1}{2}\frac{d}{dt}\iint f^2 dx dy = -\iint (f_x^2 + f_y^2) \, dx dy .$$

Why kolmogorov decay faster?

Scaling arguments show the very distinguished behavior of the kolmogorov model:

- <u>Heat equation</u>:

$$G(x,y,t) = t^{-1} F\left(\frac{x}{\sqrt{t}}, \frac{y}{\sqrt{t}}\right)$$

- <u>kolmogorov equation</u>:

$$K(x,y,t) = t^{-2} F\left(\frac{x}{\sqrt{t}}, \frac{y}{t^{3/2}}\right).$$

These structures can be discovered by scaling arguments.

- Heat equation:

If $y_t - \Delta y = 0$ then

$$y_\lambda = \lambda^d \, y(\lambda x, \lambda^2 t)$$

also solves the same heat equation.

The Gaussian heat kernel is self-similar:

$$y_\lambda = y$$

and this is equivalent to the special form

$$y = t^{-d/2} F(x/\sqrt{t}, y/\sqrt{t}).$$

- Kolmogorov equation:

The corresponding scaling is

$$f = \lambda^4 f(\lambda x, \lambda^3, \lambda^2 t)$$

and this leads to

$$f = t^{-2} F\left(\frac{x}{\sqrt{t}}, \frac{y}{t^{3/2}}\right).$$

This explains the added decay with respect to the heat equation.

In comparison with the convection-diffusion model it is natural to introduce the change of variables

$$g = f(x, y - xt, t)$$

and this time g satisfies

$$g_t - (\partial_x + t\partial_y)^2 g = 0.$$

This is a 1-d heat equation in a rotating frame.
But we also observe that the effective diffusivity increases as $t \nearrow$.

Hypocoercivity methods to achieve these decay rates are described in Villani's book following Hérau's works.

Let us first consider the heat equation.

$$y_t - \Delta y = 0.$$

Then

$$\frac{d}{dt}\left(\frac{1}{2}\int_{\mathbb{R}^d} y^2 dx\right) = -\int_{\mathbb{R}^d} |\nabla_x y|^2 dx.$$

Consider the second level energy

$$e_2 = \frac{1}{2}\int_{\mathbb{R}^d} y^2 dx + t\int_{\mathbb{R}^d} |\nabla_x y|^2$$

Then

$$\frac{de_2}{dt} = 2t\int_{\mathbb{R}^d} \nabla_x y \cdot \nabla_x y_t = -2t\int_{\mathbb{R}^d} \Delta_x y \cdot y_t$$

$$= -2t\int_{\mathbb{R}^d} |\Delta y|^2 dx.$$

We can continue:

$$e_3 = \frac{1}{2}\int_{\mathbb{R}^d} y^2 dx + t\int_{\mathbb{R}^d} |\nabla_x y|^2 dx + t^2\int_{\mathbb{R}^d} |\Delta y|^2 dx.$$

All these energies $\searrow$ as $t \nearrow$.

In particular

$$\frac{1}{2}\int_{\mathbb{R}^d} y^2 dx + t\int_{\mathbb{R}^d} |\nabla_x y|^2 dx \le \frac{1}{2}\int_{\mathbb{R}^d} y_0^2 dx.$$

And this implies that

$$\|y(t)\|_{L^2} \le \|y_0\|_{L^2}$$

$$\sqrt{t}\,\|\nabla_x y\|_{L^2} \le \frac{1}{\sqrt{2}}\|y_0\|_{L^2}.$$

These decay rates are sharp in view of the structure of the Gaussian heat kernel.

Kolmogorov rather enters in the following abstract frame very close to the discussion above on the Kalman condition for finite dimensional dissipative systems.

$$f_t + A^*Af + Bf = 0.$$

$$B^* = -B, \quad A, A^* \text{ and } B \text{ commute with } [A,B].$$

$$[A,B] \neq 0.$$

$$\|[A,A^*]x\| \le \beta\left[\|x\| + \|Ax\|\right].$$

Under these conditions

$$\|f(t)\|^2 + t\|Af(t)\|^2 + t^3\|[A,B]f(t)\|^2 \le C\|f_0\|^2.$$

Before anything, let us show that Kolmogorov enters in this abstract frame:

$$A = \partial_x, \quad A^* = -\partial_x; \quad B = -x\partial_y.$$

$$[A,B] = -\partial_x(x\partial_y) + x\partial_y(\partial_x) = -\partial_y \neq 0.$$

Obviously

$\partial_x, -\partial_x \wedge x\partial_y$ commute with ∂_y.

Furthermore: $[A, A^*] = 0 = [\partial_x, -\partial_x]$.

Thus, for kolmogorov we get,

$$\|f(t)\|^2_{L^2} + t\|\partial_x f(t)\|^2_{L^2} + t^3\|\partial_y f(t)\|^2_{L^2} \leq C\|f_0\|^2_{L^2}.$$

And these decay rates are sharp according to the structure of the kolmogorov kernel.

The proof of decay for the abstract model uses the same idea as the multi-level energies of the heat equation:

$$\frac{d}{dt}\left(\frac{1}{2}|f|^2\right) = -|Af|^2.$$

$$e_2 = \frac{1}{2}|f|^2 + t|Af|^2.$$

$$\begin{aligned}\frac{d}{dt}e_2 &= 2t(Af, Af_t) = 2t(A^*Af, f_t)\\ &= -2t|A^*Af|^2 - 2t(A^*Af, Bf)\\ &= -2t|A^*Af|^2 - 2t(Af, ABf)\\ &= -2t|A^*Af|^2 - 2t(Af, [AB-BA]f).\end{aligned}$$

In the last we have used that $B = -B^*$ and, accordingly, $(Af, BAf) \equiv 0$.

Then

$$e_3 = \frac{1}{2}|f|^2 + t|Af|^2 + t^2|A^*Af|^2 + t^2(Af, [A,B]f).$$

$$\frac{de_3}{dt} = t^2\frac{d}{dt}\left[|A^*Af|^2\right] + \frac{d}{dt}\left[t^2(Af, [A,B]f)\right].$$

With some extra effort we get to the fourth order energy

$$e_4 = |f|^2 + at|Af|^2 + bt^2(Af, [A,B]f) + ct^3|[A,B]f|^2.$$

And

$$e_4 \downarrow .$$

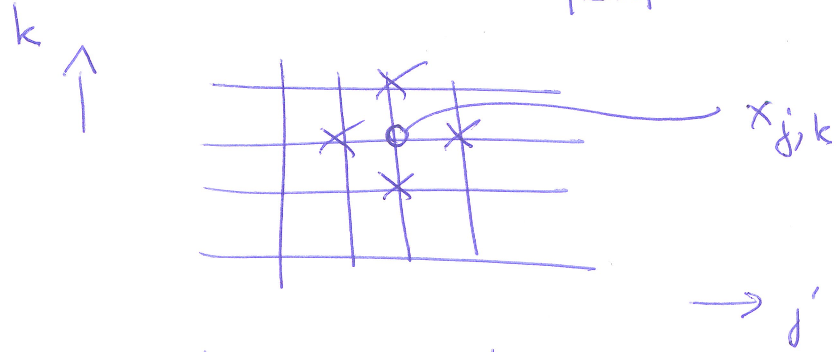
7.- NUMERICS FOR KOLMOGOROV.

We discretize

$$f_t - f_{xx} - x f_y = 0$$

$\Rightarrow$

$$f_{jk}' + 2\,\frac{f_{jk} - f_{j+1,k} - f_{j-1,k}}{|\Delta x|^2} - x_j\,\frac{(f_{j,k+1} - f_{j,k-1})}{2\Delta y} = 0$$



This is a, continuous in time, semi-discretization in space by means of finite-differences.

The key is to take centered discretization of ∂_y so to preserve its skew-adjoint structure.

This fits in the abstract frame

$$f_t + A^*Af + Bf = 0$$

with

$$A = \partial_j^+, \quad A^* = \partial_j^-$$

$$A^*A = -\partial_j^2$$

$$B = -x_j \partial_k^0$$

In the present case

$$[A,B] = -\partial_k^0$$

which provides the "hidden" dissipation of the system in the y variable in the discrete setting.

Accordingly, we recover the same decay rates for the discrete version of Kolmogorov. The discrete space-gradient energies read:

$$\Delta x \Delta y \sum_{j,k} \frac{|f_{j+1,k} - f_{j,k}|^2}{|\Delta x|^2}$$

$$\Delta x \Delta y \sum_{j,k} \frac{|f_{j,k+1} - f_{j,k-1}|^2}{|\Delta y|^2}$$

in the x and y variables respectively.

The same decay rates hold if the scheme is fully implicit in time, preserving the structure of the space-discretisation.

$$\frac{f_{jk}^{n+1} - f_{jk}^{n}}{\Delta t} + \frac{2f_{jk} - f_{j+1,k} - f_{j-1,k}}{|\Delta x|^2} - x_j \frac{f_{j,k+1} - f_{j,k-1}}{2\Delta y} = 0 .$$

8.- PERSPECTIVES.

Similar issues arise for:

* Other hypocoercive models.
Full theory of hypoellipticity due to Hormander, 68.

* Nonlinear models in kinetic theory.

REF:

A. PORRETTA & E. ZUAZUA. Numerical hypocoercivity for the Kolmogorov equation, preprint, 2015.

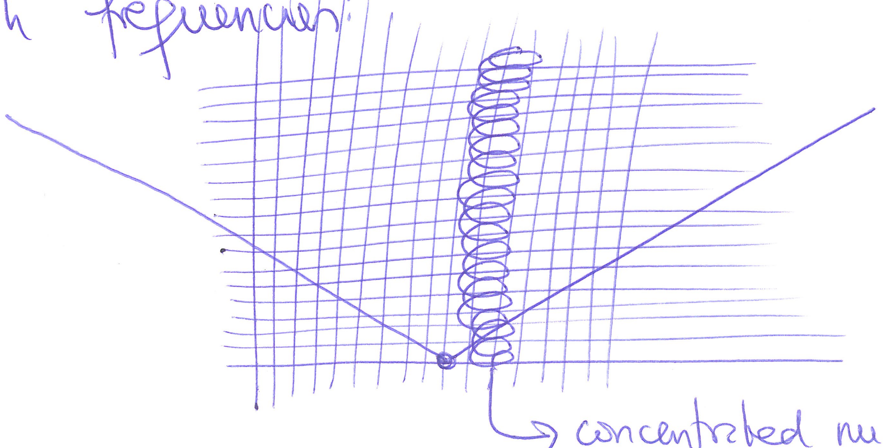
APPENDICES

• A1. Classical convergence is compatible with the lack of asymptotic preservation.

$$|y(t) - y_\Delta(t)| \leq C |\Delta t|^p e^{CT}, \; t \in [0,T].$$

For finite-dimensional systems there is an extensive literature on simplectic integration.

In the context of wave and Schrödinger equation asymptotic properties of the PDE are often lost by the numerical scheme because numerical solutions do not propagate with the appropriate speed at high frequencies.



See works by S. Ervedoza, A. Marica, E. Zuazua et al. on the subject.

- A2. A different proof of the sharp decay rate for the heat equation using Moser's iteration

$$y_t - \Delta y = 0$$

$$\frac{1}{2}\frac{d}{dt}\int |y|^2 = -\int |\nabla y|^2 \quad (\text{multiplying by } y)$$

$$\frac{d}{dt}\int |y|\,dx \leq 0 \quad (\text{multiplying by } \operatorname{sgn}(y)).$$

Assume $d=3$. Then, by Sobolev embedding

$$\left(\int_{\mathbb{R}^3} |y|^6\right)^{1/6} \leq C\left(\int_{\mathbb{R}^3} |\nabla y|^2\right)^{1/2}.$$

Thus

$$\frac{d}{dt}\int |y|^2 \leq -c \|y\|_6^2$$

But

$$\|y\|_2 \leq \|y\|_6^\alpha \|y\|_1^{1-\alpha}$$

Thus

$$\|y\|_6^\alpha \geq \frac{\|y\|_2}{\|y\|_1} \geq \frac{\|y\|_2}{\|y_0\|_1}.$$

Accordingly

$$\frac{d}{dt}\|y\|_2^2 \leq -c \frac{\|y\|_2^{2/\alpha}}{\|y_0\|_1^{2(1-\alpha)/\alpha}}.$$

This yields to sharp decay results.

This method can be further developed to get sharp decay rates $L^p \to L^q$.

This method can be adapted to deal with standard finite-difference and finite-element approximations of the heat equation.

The method can also be adapted to some non-linear models:

$$u_t - \Delta(u^m) = 0$$

$$u_t - \Delta_p u = 0$$

$$u_t - \Delta u + \operatorname{div}(\phi(u)) = 0 \ldots$$

A3. The Dirac basis

Given $f \in L^1(\mathbb{R}^d; 1+|x|)$ there exists $\vec{F} \in L^1(\mathbb{R}^d)$ s.t.

$$f = \int f \, \delta_0 + \mathrm{div}(\vec{F})$$

This expansion, although it introduces singular Dirac deltas, is useful to obtain the asymptotic behavior of the solutions of the heat equation since

$$G * f = \int f \, dx \, G + \vec{\nabla} G * \vec{F}$$

Accordingly

$$\| G * f - \int f \, dx \, G \|_p \leq C(p,d) \, t^{-\frac{d}{2}(1-\frac{1}{p})-\frac{1}{2}} \| f \|_{L^1(1+|x|)}.$$

This shows that the leading term in the asymptotic behavior as $t \to \infty$ is given by the heat kernel, since the difference decays faster, with a increased rate of the order of $t^{-1/2}$.

These expansions can be adapted and extended to any order and to the L^p-setting. The remainder term $\vec{F}$ can be expressed explicitly, providing a direct proof. But it is also interesting to observe that:

- Taking Fourier transform, we recover the Taylor expansion of $\hat{f}(\xi)$ at $\xi = 0$.
- By duality, these expansions are related to Hardy-like inequalities.

Indeed, the above identity is equivalent to

$$\int f [\varphi(x) - \varphi(0)] = \int F \cdot \nabla \varphi \quad , \forall \varphi \in C_c^\infty(\mathbb{R}^d).$$

Furthermore, obviously,

$$\left\| \frac{\varphi(x) - \varphi(0)}{|x|} \right\|_\infty \leq \|\nabla \varphi\|_\infty.$$

This is the dual version of the previous decomposition.

Classical Hardy inequalities can be employed to derive other decomposition formulas. For instance in $d=3$ we know that

$$\left\| \frac{\varphi(x)}{|x|} \right\|_2 \leq \frac{1}{4} \|\nabla \varphi\|_2 \, , \forall \varphi \in H^1(\mathbb{R}^3).$$

By duality this means that, if $f \in L^2(\mathbb{R}^3; |x|^2)$, then, there exists $F \in L^2(\mathbb{R}^3)$ such that

$$f = \operatorname{div}(\vec{F}).$$

In this case we achieve that

$$G * f = \nabla G * F.$$

Accordingly

$$\| G * f \|_2 \leq \|\nabla G\|_1 \|F\|_2 \leq t^{-1/2} \|F\|_2$$

This shows that the added integrability at infinity ($f \in L^2(\mathbb{R}^d; |x|^2)$) induces a gain on the decay of the order of $t^{-1/2}$.

14. Similarity variables

The equation
$$u_t - \Delta_x u = 0$$
can be rewritten as
$$v_s - \Delta_y v - \frac{y \cdot \nabla v}{2} - \frac{d}{2} v = 0$$
in the new space-time variables
$$s = \log(t+1) \; ; \; y = x / (1+t)^{1/2}$$
and with
$$v(y,s) = e^{sd/2} u(e^{s/2} y, e^s - 1).$$
This new heat equation in the similarity variables can also be written in the following symmetric form
$$k(y) v_s - \mathrm{div}_y \left(k(y) \nabla_y v \right) - \frac{d}{2} v = 0$$
with
$$k(y) = \exp(|y|^2/4).$$
This equation can be analyzed in the context of weighted spaces $L^2(k)$; $H^1(k)$. It is noteworthy that the embedding $H^1(k) \hookrightarrow L^2(k)$ is compact. The spectral decomposition is also explicit and this leads to a complete asymptotic expansion, similar to the one achieved in the Dirac basis.

These issues were systematically developed in the works by M. Escobedo, O. Kavian & E.Z.