DIFFERENTIAL EQUATIONS ON GRAPHS

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Abstract. We look at examples of dynamical systems on finite simple graphs. These systems correspond to partial differential equations in the continuum. This documents contains some notes related to a project supported by the HCRP Summer 2016 program with Annie Rak who submitted in November 2016 a senior thesis about advection, a particular aspect of this PDE topic.

1. Introduction

1.1. Most **partial differential equations** on a compact Riemannian manifold M are formulated in terms of an exterior derivative d given on M. A Riemannian metric on M then defines inner products on k-forms and so dual notions d^*. Of particular interest are the Laplacians $L_k = d_k^* d_k + d_{k-1} d_{k-1}^*$ which define **Laplace equations** $L_k u = 0$, **Poisson equations** $L_k u = g$, **heat flows** $u' = -L_k u$ or **wave equations** $u'' = -Lu$ all defined on k-forms. Examples of nonlinear equations are the sin-Gordon equation $u'' = -Lu + \sin(u)$ or the **eiconal equation** $|df| = 1$ on k-forms. Among linear systems, also the **advection transport equations** like $u' = d_v^* du$ or $u' = d^* d_v u$ are of interest, where d_v rsp. d_v^* are modifications of d, d^* playing the role of a generalized gradient or divergence and where v is a vector field, defined by a weighted edge attached to a vertex.

1.2. Since classical PDEs only refer to an exterior derivative, a translation to the discrete should be straight forward. In particular, an adaptation to graphs where a natural exterior derivative and calculus exists using incidence matrices as defined by Poincaré. One should note however that discrete differential calculus has been initiated half a century before Poincaré already starting with Kirchhoff who is commemorated in the Laplacian L on a graph: one often calls this matrix the **Kirchhoff operator**. Some of the discretizations, especially in

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the nonlinear realm are not canonical at all. One would like to emulate the continuum as well as possible. Discretizations of nonlinear systems in particular should have global existence results if the continuum version has global solutions. The discrete versions also should preserve integrability. The discretization should also work for general networks and not only for numerical discretisations of continuum spaces. Still, already in the linear case we would like to have a match between the behavior on discrete spaces and the continuum limit without just doing numerical discretizations in the form of partial difference equations. In the discrete, on a general network, functions on the set of k-dimensional simplices play the role of k-tensors. After a pre-ordering of the simplices, one can define anti-symmetric tensors, discrete analogue of k-forms. Following Poincaré, the exterior derivatives are then given by **incidence matrices** of the graph. While the Laplacians are independent of the choice of directions, the prescribed orientations in general matter. The classical transport equation $u_t = u_x$ for example on k-forms, needs to be replaced by $u_t = Fdu$, where F is a suitable operator from $(k+1)$-forms to k-forms. If $F = -d^*$, transport happens in all directions, leading to diffusion. For $F(u)(v) = u(G(v))$ with a vector field G assigning to a vertex v an edge $G(v)$, then this is deterministic transport and a flow analogue to a differential equation $u' = G(u)$ on a manifold M, where G is a vector field, a map $x \to G(x) \in T_xM$ from M to the tangent bundle of M.

1.3. When looking at evolution equations in a discrete set-up, one has to make some choices: one can discretize **space**, **time** or the **target space** of the functions. In this project, we assume space to be discrete. Rather than quantizing time also, we consider **difference-differential equations** of the form $u_t = A(u)$ with a discrete difference operator defined by possibly modified incidence matrices, leading to exterior derivative d and operators $D = d + d^*$ or $L = D^2$. If a time derivative is involved, these equations become **ordinary differential equations** with finitely many variables. What about time and target space discretisations? A time discretisation in general is no problem, as on a fundamental level, one can just deform the polynomial algebra to get the same formalism as in the continuum. We don't go into this quantum calculus frame work here (known to Newton, Gregory and Taylor already) but roughly, it works as follows: the time derivative d/dt is replaced with a difference operator like $Df(t) = f(t+1) - f(t)$. Now, if the polynomials are deformed such that $Dx^n = nx^{n-1}$ and the exponential function is redefined so that $De^{ax} = ae^{ax}$ (there is canonical way to do that like $[x]^2 = x(x-1)$

so that $D[x]^2 = (x+1)x - x(x-1) = x2 = 2[x]$ etc or by defining $e^{ax} = (1+ax)^n$ so that $e^{a(x+1)} - e^{ax} = ae^{ax}$), we don't have to change the content of calculus books. The original intentions of the calculus books is then just the limiting idealized case, where one deals with smooth functions). For more details, see [5]. Like Nelsons non-standard analysis [9], the discrete setup is an extension of the traditional calculus as we know and teach it. The results remain true verbatim: its just that the meaning of the formulas has changed. So, discretizing time is no problem on a fundamental level. Discretizing the target space is more subtle and serious, as it leads to cellular automata [12], where the adaptations of the models is often not obvious: the task for example to build cellular automaton for which solutions behave like the wave equation is more subtle if the target space is just a finite set but it is done already on a computer as a computer always deals with functions taking finitely many values, but where the computer also produces some unpredictable noise due to rounding arithmetic. The investigation of finite dynamics obtained by simulating continuum systems has been pioneered in the 70ies already [10] and was studied since. Examples are [13, 7]. So, in the following, we assume space is a graph, time is the real axes and the functions are real-valued.

2. Examples

2.1. The **Heat equation** on k-forms is the dynamical system

$$u_t = -Lu$$

on k-forms, where L is the Laplacian on k forms. It produces the **heat flow**. Since L is just a finite matrix, it can be solved directly with $e^{-Lt}u(0)$ or by doing an eigenvalue expansion $u(t) = \sum_{j \in \mathbb{Z}} \hat{u}_j e^{-\lambda_j t} f_j$. The set Ω^k of k-harmonic functions is the attractor on Ω^k. In the case $k = 0$, these are the functions which are constant on connected components. The flow is geometrically interesting on $\Omega = \bigcup \Omega^k$ as in general the super trace $\text{str}(L) = \sum_k (-1)^k \text{tr}(L_k)$ stays constant by McKean-Singer. This implies that the super trace $\text{str}(e^{-Lt}) = \sum_{k\text{even}} tr(e^{-L_k t}) - \sum_{k\text{odd}} \text{tr}(e^{-L_k t})$ is constant. The energy $E(u) = \sum_{x \in V} u(x)^2 = \langle u, u \rangle$ is always a **Lyapunov function** on any space Ω^k of differential forms: it decreases as $E'(u) = \langle -Lu, u \rangle = -\langle dd^* + d^*du, u \rangle$ which is $-\langle d^*u, d^*u \rangle - \langle du, du \rangle = -|d^*u|^2 - |du|^2 \leq 0$.

2.2. Given an initial position and velocity, the **wave equation**

$$u_{tt} = -Lu$$

has the explicit **d'Alembert solution** $\cos(Dt)u(0)+\sin(Dt)D^{-1}u'(0)$, where $D = d+d^*$ and D^{-1} is the inverse matrix restricted to the ortho-complement of the kernel. We see that it is really useful to look at the wave equation simultaneously on all forms Ω^k since there, the Laplacian L has a factorization $L = D^2$. Because D is a non invertible matrix, the initial velocity $u'(0)$ must be chosen perpendicularly to the kernel of D. The inverse D^{-1} can then be understood as the **Moore-Penrose inverse** of D: we only invert on the subspace spanned by eigenvectors to non-zero eigenvalues. In the case of scalar functions, we only need the velocity to average to zero. The solution can also be obtained by going into a basis in which L is diagonal. If $u(0) = \sum_k \hat{u}_k f_k$ and $u'(0) = v(0) = \sum \hat{v}_k f_k$ and $Lf_k = \lambda_k f_k$, then

$$u(t) = \sum \hat{u}_k \cos(\sqrt{\lambda_k} t) f_k + \hat{v}_k \sin(\sqrt{\lambda_k} t)/\sqrt{\lambda_k} f_k \ .$$

The wave equation has the integrals of motion $\hat{u}_k^2+\hat{v}_k^2$ and is an example of a Hamiltonian system. On each eigen-mode, we have a **harmonic oscillator**. The wave equation therefore is equivalent to a product of finitely many harmonic oscillators. This is the same in the continuum, but only that the number of oscillators is now countable. A Fourier expansion renders the wave equation equivalent to a sequence of harmonic oscillators. Now, the d'Alembert solution can be implemented fast numerically if the matrix exponential has been built in. Computer algebra systems have procedures like matrix exponentiation already hardwired so that solving the wave equation on a general network needs only a few lines of code.

2.3. The **Laplace equation**

$$Lu = \lambda u$$

is just an eigenvalue problem for the form Laplacian L. For $\lambda = 0$, the solutions are called **harmonic forms**. There are solutions to the Laplace equation if and only if λ is an **eigenvalue** of L. This motivates to study the eigenvalues of the operators L_k on k-forms. As mentioned already, these spectra have some Mc-Kean Singer symmetry: the union of the eigenvalues on even forms is the union of the eigenvalues on odd forms. [8, 4] The inverse spectral theorem is to find the set of graphs for which the form spectra are the same. There are many examples known of this type. The structure of the solutions is of interest too. For any eigenfunction, one can look the **nodal surfaces**, graphs formed by complete subgraphs on which function changes sign [6].

2.4. Also the **Poisson equation**

$$Lu = g$$

is in finite dimensions just a linear algebra problem. For g perpendicular to the kernel of L, this has a solution $u = L^{-1}g$, where L^{-1} is the pseudo inverse. Many problems in physics can be formulated as Poisson equations. Here are two examples: the Poisson equation $LA = j$ on 1-forms for example has an interpretation as a **Maxwell equation**: think of j as the current and of A as the **electro magnetic potential**. If A is gauged (replaced by $A + df$) so that $d^*A = 0$, then $F = dA$ and $j = LA = (d^*d + d^*d)A = d^*dA = d^*F$ it gives the **Maxwell equations** $dF = 0, d^*F = j$. The Poisson equations also give the force F from the mass density ρ as $LF = \rho$ is the **Gaussian formulation of gravity**. In $\mathbb{R}^3$ with a spherically symmetric spherically symmetric charge distribution of compact support, it produces the Newton force C/r^2 away from that support, where r is the distance to the center of the charge and C is a constant which depends on the mass of the body.

2.5. Like the Laplace or Poisson equation, the **eiconal equation** is not a time evolution. It is the discrete difference equation

$$|du| = 1$$

where $|du(x)|$ is the maximal absolute value of the derivative du on $k+1$ forms attached to the simplex x. For $k = 0$, the Eiconal equation tells that all gradients are constant 1. It is nonlinear in nature as in the continuum; in Euclidean space R^3 for example it is $f_x^2 + f_y^2 + f_z^2 = 1$. Already in the continuum, on simple surfaces like ellipsoids, the solutions fail uniqueness on caustics defined by the initial condition. The structure of these caustics is still in the dark even for ellipsoids and initial Dirac initial conditions located on a point, where Jacobi's last statement on caustic is an open problem. In the discrete, the solutions of the eiconal equations are k-forms with the property that the maximal steepness at every k-simplex x is 1. This interpretation is motivated by the fact that in the continuum, the maximal directional derivative at a point is the length of the gradient. Let a graph be **flat** if the distance function to any point satisfies the eiconal equation globally. Examples of flat graphs are wheel graphs with less than 7 vertices or trees or the hexagonal tiling graph in the plane, where each vertex has 6 neighbors. Can we characterize graphs which admit a global solution to the eiconal equation?

2.6. Convection. Replace the adjoint d^* in $u_t = -d^*du$ or $u_t = -dd^*u$ or $u_t = -Lu$ with an other operator from $(k+1)$-forms to k forms. An example for $k = 1$ is

$$u_t = d(v \cdot u)$$

which is a differential equation on 1-forms. Here v is a fixed 1-form and $v \cdot u$ is the dot product defined as $v \cdot u(x) = \sum_{(y,x) \in E} v(y)u(y)$. One can think of v as a background field which guides the diffusion. It for example applies if a graph is weighted. Think of $v(e)$ as how much can get through the edge e. The sum $\sum_x u(x)$ is conserved under the time evolution simply because its derivative is a sum over gradients.

2.7. Advection. We could also look at the system

$$u_t = v \cdot du$$

on 0 forms. Here again, v is a fixed **background direction** 1**-form**. This allows to model the flow of a "vector field" v. This is a modification of $u'(i) = \sum_j F(e)du(e)$. If $L_+ = B_+ - A$, where B_+ is the **out vertex degree matrix** and A is the adjacency matrix. Now, $u' = -L_+u$. There is a dual **consensus dynamics** $u' = -L_-u$ and of course **diffusion dynamics** $u' = -Lu$ which is the heat equation. The sum $\sum_{x \in V} u(x)$ is conserved. [1] look at $u'(i) = \sum_j v(j \to i)u(j) - \sum_j v(i \to j)u(i) = (D^v - A^v)u$. Here, $v(i \to j)$ is a function attached to the directed edge $i \to j$. The right hand side can be written as d^*vd_0, where $d_0 = \max(d, 0)$ and d is the exterior derivative. Compare that d^*vd is a weighted graph Laplacian.

2.8. The **Sine-Gordon equation** is

$$u_{tt} = -Lu - c\sin(u)$$

In the simplest case of a one-point graph $G = K_1$ we have the physics **pendulum** $u_{tt} = -c\sin(u)$, one of the simplest nonlinear Hamiltonian systems. In the case of the complete graph with two vertices K_2, we have the Hamiltonian differential equation

$$x''(t) = -x(t) + y(t) - c\sin(x(t)), y''(t) = -y(t) + x(t) - c\sin(y(t)) .$$

It defines a flow on a 3-dimensional energy surface which we measure to be integrable: the orbits appear to lie on tori. For $c = 0$, it is a flow on a three sphere. Also for small c, the energy surface is still a topological sphere and we expect the flow to remain integrable in the sense that all orbits are located on points or 1D or 2D tori. Numerics confirms that. Can this be written as a Lax pair as in the case of the pendulum? The three dimensional energy surface $H(x,y,x',y') = (x'^2+y'^2)/2 + (x-y)^2/2 + \cos(x) + \cos(y)$ is constant. For a circular graph $G = C_n$, the stationary points of the sin-Gordon equation are critical points of the Frenkel-Kontorova model and correspond to periodic solutions of a symplectic map, the **Standard map** given by the second order recursion equation $x_{n+1} - 2x_n + x_{n-1} = c\sin(x_n)$ leading to the map $(x,y) \to (2x - y + c\sin(x), x)$ on the 2-torus $\mathbb{R}^2/(2\pi\mathbb{Z})^2$.

2.9. Burgers equation. The classical friction-free Burgers equation on the real line $u_t = 2uu_x$ can be written as $u_t = (u^2)'$, where u' is the gradient. If u is a function which vanishes at infinity or is defined on a circle, this differential equation classically has the integral $F(u) = \int_R \log(u)\, dx$ as $F'(u) = \int_R u_t/u\, dx = \int_R u_x\, dx = 0$. In the discrete, we can define an operator $F : \Omega^k \to \Omega^{k+1}$ which assigns to a form u the form $F(u)(x) = S(\sum_{y,z \subset x} u(y)u(z))$, here S anti-symmetrizes, which is only necessary for $k > 0$. Now we can look at the differential equation

$$u' = d^* F(u) \quad .$$

As an example, lets consider at the case of a circular graph $C_n = (V,E)$ and a 0-form u, for which $F(u)((a,b) \in E) = u(b)u(a)$. Now, $d^*F(u)(n) = u(n)(u(n+1) - u(n-1))$. The differential equation is well studied and called the **Volterra-Kac-Moerbeke Langmuir lattice**

$$u_t(n) = u(n)[u(n+1) - u(n-1)] \ .$$

It is integrable and equivalent to the **Toda lattice** [11]. What happens on a general graph? Is it still integrable?

2.10. Navier Stokes type equations. Assume u is a function on edges modeling a velocity field and that we have a pressure 2-form $p(u)$, a stress tensor $T(u)$ and a tensor product $u \oplus u$ and a force term F which is a 1-form, a discrete Cauchy momentum equations is $u' + d^*(u \oplus u + p) = d^*T + F$. To make sense of this in the discrete, we need a cross product on graphs and a notion of pressure. Since pressure is defined as $F = pA$, where A is the area element and F the force, we could define $u \oplus v$ as $\sum_{i,j} u_i v_j$, where i,j runs over all pairs of edges in the triangle t. If we think about T as the adjacent pressure functions, then $(u \oplus u + p - T)(t)$ could be modeled more easily as a function on triangles given by summing u over all edges hitting the triangles but not being in the triangle, then summing over all pairs (e, f) of edges in the triangle t and then over all pairs of edges not in the triangle. The most natural simplification is $u' = d^* F(u)$, where $F(u)(t) = \sum_{e,f \subset t} u(e)u(f)$ is a nonlinear 2-form, a function on triangles. One can generalize this to differential equations on k-forms:

$$u' = d^* \sum_{e,f} u(e)u(f)$$
,

where the sum $F(u)(x)$ on a $(k+1)$ simplex x sums over all pairs of k-simplices which intersect. This is not yet explored at all, but it could be that "fluid dynamics" in a connection calculus setup on a network can be set naturally. In the continuum, the difficulty is illustrated by the struggle to see whether global solutions exist.

3. Wave speeds

Since $L = D^2$, the wave equation $(d^2/dt^2 + L)\psi = 0$ can be factored $(d/dt + iD)(d/dt - iD)\psi = 0$ leading to the **Schrödinger equations** $\psi' = \pm iD\psi$ for the Dirac operator D and a complex-valued function $\psi(t) = u(t) + iD^{-1}u'(t)$ encoding position $u(t) = \mathrm{Re}(\psi(t))$ and velocity $u'(t) = D\mathrm{Im}(\psi(t))$ of the classical wave. We write $\exp_x(v) = \psi(t)$ if $\psi(0) = x + iD^{-1}v$. One of the basic questions we would like to know is how fast signals propagate on the space of k-forms. We have not yet looked at this systematically.

4. Integrability

A differential equation is **DS integrable**, if every invariant measure defines an almost periodic systems in the sense that the spectrum of the Koopman operator has pure discrete spectrum [2]. In smaller dimensional systems, this can be the case if every invariant measure of the flow is located either on a fixed point, a fixed circle, a fixed 2-torus or higher dimensional torus and the dynamics is conjugated there to a translation. The pendulum is an example the flow is integrable as every invariant measure is either located on an equilibrium point or a one dimensional circle (homotopically trivial for small energies and wrapping around the cylinder phase space for larger energies). The heat and wave equations are examples of integrable systems when considered on graphs: For the heat flow, every invariant measure is located on a point, a constant function, for the wave flow, every invariant measure is located on a torus. The dimension depends on rational dependencies of the scaled eigenvalues $2\pi\lambda_k$ of the Dirac operator $D = d + d^*$ of the graph.

A special case of the just given notion of integrability is **Liouville integrability**. Recursively, a system can be called Liouville integrable if it is defined on a finite dimensional manifold M, for which there exists a smooth invariant function (Liouville integral) such that on every level set $\{f = c\}$ the system is again Liouville integrable. Liouville integrability implies integrability in the above sense but the reverse is not known. One could imagine invariant sets on which the dynamics is conjugated to a group translation on an other compact group than a torus. But no such example seems to be known. The problem is related to the problem to determine whether there are open sets of Hamiltonian systems of dimension $d \geq 4$ on which no weak mixing tori exist; it is not known whether open sets of smooth integrable Hamiltonian systems exist in dimension larger than 2, if integrability is understood in the above sense (using invariant measures).

There are many notions of "integrable". Birkhoff for example suggested an analytic version in that that the phase space is partitioned into regions, in which the Birkhoff normal form at an equilibrium point converges. This is probably not equivalent since it can happen that in touching boundaries of different regions of analyticity the dynamics is chaotic. Such phenomena happen in complex dynamics, where on the boundary of a Siegel disk or Herman ring the dynamics can be chaotic. No such phenomena are known in say more narrow classes of systems like Hamiltonian systems. Even the classic Kolmogorov problem on mixing invariant tori (which initiated research on KAM theory initially) is open. See [3].

5. Topology

Differential equations on graphs help to prove theorems. Here is an example, where the heat flow is used to prove the Brouwer-Lefschetz fixed point theorem. A special case of this theorem tells that if a graph G is homotopic to a point, then any automorphism of G necessarily has a fixed simplex. Since a simplex is a vertex of the Barycentric refinement and the Barycentric refinement of a graph has the same cohomology, this easily implies the classical Brouwer-Lefschetz fixed point theorem.

Lets first look at the cohmology. Since the exterior derivative satisfies $d^2 = 0$, the kernel of $d_p : \Omega^p \to \Omega^{p+1}$ contains the image of d_{p-1}. The vector space

$$H^p(G) = \ker(d_p)/\mathrm{im}(d_{p-1})$$

is the p'th **simplicial cohomology** of G.
The **Betti numbers** $b_p(G) = \dim(H^p(G))$ define $\sum_p (-1)^p b_p$ which is **Euler characteristic** $\chi(G) = \sum_x (-1)^{\dim(x)}$, summing over all complete subgraphs x of G. If T is an automorphism of the graph G, the **Lefschetz number**, the super trace $\chi_T(G)$ of the induced map U_T on $H^p(G)$ is equal to the sum $\sum_{T(x)=x} i_T(x)$, where $i_T(x) = (-1)^{\dim(x)}\mathrm{sign}(T|x)$ is the **Brouwer index**. This is the **Lefschetz fixed point theorem**:

For $T = Id$, the Lefschetz formula is **Euler-Poincaré**. By Hodge theory, $b_p(G)$ is the nullity of L restricted to p-forms. By **McKean Singer super symmetry**, the positive Laplace spectrum on even-forms is the positive Laplace spectrum on odd-forms. The super trace $\mathrm{str}(L^k)$ is therefore zero for $k > 0$ and $l(t) = \mathrm{str}(\exp(-tL)U_T)$ with $U_T f = f(T)$ is t-invariant. This heat flow argument proves Lefschetz because $l(0) = \mathrm{str}(U_T)$ is $\sum_{T(x)=x} i_T(x)$ and $\lim_{t\to\infty} l(t) = \chi_T(G)$ by Hodge.

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