PROJECT OUTLINE

Indicate the state of the art.

This project is concerned with imprecise Markov chains: robust generalisations of Markov chains, based on the theory of imprecise probabilities. In this state of the art section, we briefly introduce Markov chains and imprecise probabilities, explain how they can be combined to obtain imprecise Markov chains, and then go on to give an overview of recent advances in this field.

Markov chains

A *discrete-time finite-state Markov chain* is a special stochastic process. It models the time evolution in discrete time steps of a system that can be in a finite number of states. It is *stochastic* because the model is given in terms of probabilities, such as, for example, the probability to be in a certain state at a given time. It is a Markov chain because the probabilistic model satisfies a *Markov condition*: the (so-called) transition probability to be in a certain state at the next time step only depends on the current state, and not on the past states. The probabilistic time evolution of the state of such Markov chains is described by linear difference equations. In *continuous-time Markov chains*, the time steps become infinitesimally small, and their time evolution is described by linear differential equations. Both discrete and continuous-time Markov chains belong to the most powerful, and—due to their reasonable computational complexity—the most widely used probabilistic models in a very wide range of applications in engineering (filtering, control, queueing), AI (text and speech recognition), mathematical finance and bio-informatics, to name only a few domains.

Imprecise probabilities and the limitations of precise models

Nevertheless, these Markov chains have limitations: we will focus here on two of them. The first is that the uncertainty about the state is described by (transition) probabilities: real numbers whose precision is almost always unwarranted in applications, because of the limited accuracy and reliability of statistical estimation methods, and the essentially limited numerical accuracy that computer simulations offer. The second limitation is related to the Markov condition: that the probabilistic model for the next state depends only on the current one, is quite a strong assumption to make. It leads to a drastic decrease in computational complexity, and is therefore often made, but is typically hard to justify in practical applications. The justification that is commonly given for both of these assumptions in modelling contexts is that the simplification they entail is unlikely to have major implications for the conclusions that we draw from the models. However, this claim is hard to verify, and often unwarranted. As a brief look at the mathematics of these stochastic models will already show, there are many situations where (i) the conclusions of a Markov chain analysis depend heavily and crucially on the precise values of the transition probabilities, or where (ii) not making a Markov assumption leads to qualitatively very different results.

Interestingly, in recent decades much progress has been made in extending the existing corpus of general probabilistic knowledge to deal with both types of limitations: the field of *imprecise probabilities* [1,15, 26] has, amongst other things, developed well-justified, mathematically rigorous, as well as robust and efficient methods for dealing with both of them. Stated in very simple terms, an imprecise probability model is a probabilistic model that is partially specified. For example, whenever it is infeasible to reliably estimate the probability of some event, the theory of imprecise probabilities allows for the use of a probability interval instead. Such partial specifications do not lead to a unique probability measure, but instead give rise to a set of compatible probability measures. These sets of probability measures are called credal sets. They are the basic uncertainty models in imprecise probability theory. A credal set can be represented equivalently by a so-called *lower expectation*: a non-linear operator that is the lower envelope of the linear expectation operators associated with the probability measures in the credal set. Remarkably, the state of the art in the theory is able to perform the necessary robust calculations and derivations for all of the (infinite number of) precise probability measures in such a credal set, with a computational efficiency that is not much lower than—and often as low as—the one for the precise models; see for instance [3, 5, 8, 9] for concrete examples that substantiate this claim.

A brief introduction to imprecise discrete-time Markov chains

Applying the results and ideas developed in the field of imprecise probabilities has led to interesting advances in *discrete-time* finite-state Markov chains, resulting in a theory of so-called *imprecise Markov chains* [6, 9–11, 25]. They correspond to a collection of stochastic processes that are only 'superficially Markov', in the sense that their *sets* of transition probabilities satisfy a Markov condition, whereas the individual members of those sets need not. Imprecise Markov chains are *not* simply collections of precise Markov chains, but rather correspond to collections of general stochastic processes whose transition models belong to sets that satisfy a Markov condition. In this sense, they lead to more robust and reliable inferences than their precise counterparts, and nevertheless still allow for very efficient and elegant computations, a combination that is clearly important in applications.

Imprecise probability trees and submartingales

A crucial step that made these developments possible was the observation that general discrete-time stochastic processes can be described elegantly using probability trees: graphs whose *paths* from root to leaves represent possible time evolutions of the process, whose nodes (called *situations*) represent time evolutions up to a certain time step, and where each situation has a local probability model for what may happen at the next time step. The paths correspond to the elements of the sample space in the more conventional measure-theoretic approach. With such a tree there is associated a convex closed set of so-called martingales—real processes with zero expected increase from one time step to the next—and an important result by Ville [13, 17] shows that all probabilistic properties of, and inferences about, the stochastic process are completely determined by this set of martingales. Going to imprecise stochastic processes now becomes fairly straightforward, at least conceptually: the local models in the tree's nodes are now sets of probabilities, and all probabilistic inferences are, through an extension of Ville's Theorem, characterised by the corresponding convex closed set of *sub*martingales (real processes with non-negative expected increase under all precise probability models in these sets) [6, 7].

State of the art for discrete-time imprecise Markov chains

There have been several approaches to extending Markov chain theory to deal with imprecision. Hartfiel [10], using the name *Markov set-chains*, focussed on lower and upper bounds for the transition probabilities between individual states, and also discussed sets of transition operators, recognising the importance of convexity of sets of distributions over states, separately specified rows and coefficients of ergodicity. Unaware of Hartfiel's work, Kozine and Utkin [12] proposed an approach with a different underlying interpretation, and very different computational aspects. Instead of allowing transition probabilities to vary within given bounds from one time step (or state) to the next, they assumed a single precise but unknown Markov model: they worked with sets of precise Markov chains.

The first systematic and fully rigorous approach to combining discrete-time Markov chains with imprecise probabilities is due to De Cooman et al. [9], using the idea of lower conditional expectations—also called lower transition operators. Similar ideas were explored independently by Škulj [20], who focussed instead on interval probability models and their associated convex sets of probability distributions. For calculations and inferences, the main difference between the two approaches is that the lower transition operator approach in [9] allows for very efficient backwards induction, in contrast with the much less efficient forward calculations typical in the sets of distributions approaches [20]. Lower transition operators, and the ideas used in the analysis of the limit behaviour of imprecise Markov chains, introduced in [9], became the basis for most of the later work on imprecise Markov chains. They also emerge naturally as special cases in the above-mentioned theory of imprecise stochastic processes based on imprecise probability trees and closed convex sets of submartingales [6].

One topic that has been studied extensively, is the limit—or stationary—behaviour of imprecise Markov chains, which is very important and useful when looking at practical applications. Necessary and sufficient conditions for convergence to a unique attractor, expressed in terms of properties of transition operators, were studied by De Cooman and Hermans [9, 11]: although such convergence seems easier to attain for imprecise Markov chains, its characterisation becomes rather more involved. Škulj and Hable [25] characterised unique convergence in terms of coefficients of ergodicity: in addition to providing conditions for convergence, these also measure its rate. When there is no unique attractor, imprecise Markov chains display a very different behaviour from precise models. The analysis of accessibility between states becomes much more complicated, as does the analysis of the structure of invariant imprecise distributions. Škulj [21] provided a general classification of such invariant distributions. Also practically useful is the so-called conditional convergence for Markov chains with absorbing states and certain absorption: in the long run the chain will be absorbed into the absorbing state, but, under regularity assumptions, the distribution conditional on the event that the chain has not yet been absorbed converges to a stationary distribution. For imprecise Markov chains, Crossman and Škulj [2] proved the existence of a unique imprecise stationary conditional distribution under regularity assumptions.

More recent work has begun to address other practically useful properties of imprecise discrete-time Markov chains. Škulj [23] uses coefficients of ergodicity to measure the sensitivity of imprecise Markov chains to perturbations in its parameters. A systematic study of expected time to absorption, expected return times, stopping times, hitting probabilities, and ergodicity was initiated in [6, 14], but a complete theory is still under development. Time reversal and reversible Markov chains rely on specific properties of transition operators and stationary distributions that turn out to be quite hard to extend to their imprecise versions. Although a complete description of reversible processes is not yet possible, a first successful attempt was made by Škulj [24], by studying a special family of reversible imprecise Markov chains that are obtained as random walks on weighted graphs.

State of the art for continuous-time imprecise Markov chains

The discussion above, as well as the bulk of the literature on imprecise Markov chains, deals mainly with their discrete-time variant: very little is known about how to deal with robustness and imprecision in continuous-time Markov chains. Imprecise continuous-time Markov chains can be related—be it rather artificially—to continuous-time Markov decision processes and controlled Markov chains; these notions share the basic idea of multiple possible transition scenarios. Addressing them using the ideas and efficient techniques of imprecise probabilities has only been attempted very recently [4,16,22]. Many basic conceptual, theoretical and computational problems have yet to be solved, and the relationship with the continuous-time versions of imprecise probability trees and closed convex sets of submartingales has yet to be explored. So far, Škulj [22] has used ideas from the discrete-time approach to introduce imprecise versions of transition rate matrices and establish an appropriate counterpart for Kolmogorov's backward equation, leading to a non-linear differential state evolution equation. He proved that it has maximal and minimal solutions that characterise all possible solutions. Finding these boundary solutions numerically is still very much a problem under study, but has huge potential for practical applications.

Describe the objectives of the research.

Describe the envisaged research and the research hypothesis, why it is important to the field, what impact it could have, whether and how it is specifically unconventional and challenging.

The main objective of the proposed research project is to make significant progress in the development of the theory of imprecise *continuous-time finite-state* Markov chains, using recent developments in imprecise probabilities [1, 15] and imprecise probability trees [7, 13], and building on what has already been achieved in the discrete-time case [6, 9, 11, 25]. In particular, we want to develop the following three lines of research; more detailed information is provided in the Methodology section below.

- Develop a rigorous martingale-theoretic and measure-theoretic definition for the joint model of a continuous-time imprecise Markov chain, and use this model to generalise a number of basic theoretical properties of precise continuous-time Markov chains.
- Develop computational methods for imprecise continuous-time Markov chains and conduct a theoretical analysis of their efficiency, with a particular focus on convergence speed (coefficients of ergodicity) and stability (perturbation analysis).
- Study and characterise the limit behaviour of imprecise continuous-time Markov chains: "Under which conditions will they converge to a stationary limit distribution?", "What properties does such a limit distribution have?" and "How can we efficiently compute it?".

Over the past decades, similar lines of research have received plenty of attention for *precise* continuous-time Markov chains, and this has resulted in their successful application in various domains, including control engineering, queueing, artificial intelligence, bio-informatics and survival analysis. However, for *imprecise* continuous-time Markov chains, these topics are almost completely unexplored. Our research hypothesis is that by developing these three lines of research, it will become technically feasible to successfully apply imprecise continuous-time Markov chains to the same types of problems that are currently solved with their precise versions, and provide them with more robust solutions.

Indeed, the practical advantage of our 'imprecise' approach is that it explicitly acknowledges that we may not know the relevant probabilistic models exactly, and that, as a result, our inferences must be robust against such model uncertainty. The framework of results and inference methods to be developed will be able to predict the effect of this model uncertainty on specific interesting functions of state variables, for example by providing lower and upper bounds on their expectations. The results of such inferences can then be used in various applications and situations, for instance to make safer design choices that are more robust against modelling errors.

The proposed research is unconventional from the perspective of both domains that intersect in this project. From the point of view of Markov chain theory, it is unconventional because it does away with two traditional assumptions: the Markov condition is replaced by a weaker version, and the probabilities that make up the model do not have to be specified exactly. And from the imprecise probability perspective, this project is unconventional because time is taken to be continuous, whereas past research on imprecise stochastic processes has focussed almost unanimously on discrete-time problems.

Due to the unconventional nature of the proposed research, and because the topic is largely unexplored, the project will clearly be challenging. However, given the extensive experience of both partners in studying various aspects of imprecise *discrete-time* stochastic processes [6, 7, 9, 11], we are convinced we have the necessary expertise to successfully tackle similar research problems in continuous time.

Describe the methodology of your research.

Be as detailed as necessary for a clear understanding of what you propose. Describe the different envisaged steps in your research, including intermediate goals. Indicate how you will handle unforeseen circumstances, intermediate results and risks. Show where the proposed methodology is according to the state of the art and where it is novel. Enclose risks that might endanger reaching project objectives and the contingency plans to be put in place should risk occur.

As explained in the objectives section, we intend to pursue three lines of research, each of which has been very successful for precise continuous-time Markov chains, but none of which has so far seen significant progress in the imprecise case; a detailed plan for each is outlined below. Each research line will initially be carried out by a dedicated full-time PhD student, under the close supervision of the (co-)supervisors and a part-time senior researcher. As time and research progresses, we expect these research lines to benefit from each other, leading to intensive collaborations between the respective students (and their supervisors). Concrete topics for collaboration are discussed within the following detailed plans.

Joint models and basic properties **(Research Line 1)**.

A first important goal of this project is to develop a rigorous martingale-theoretic and measure-theoretic definition for the joint models of a continuous-time imprecise Markov chains, and to use these models to generalise a number of basic theoretical properties of precise continuous-time Markov chains. This research can be divided into the following three work packages.

- The first step will consist in *investigating how to define an imprecise probability tree, and in particular an imprecise Markov chain, in continuous time*: what are the possible paths and nodes, how can we define local imprecise probability models attached to these nodes, and how do we formulate a Markov condition for them? In addition, it must be investigated how to define the submartingales associated with such a continuous-time imprecise probability tree, and whether and how this definition simplifies when we impose the Markov condition **(Work Package 1a)**. To achieve this, we can draw inspiration from earlier game-theoretic probability work done by Vovk in characterising the (precise) probability tree associated with continuous-time Brownian motion [18, 19], a special case of a Markov chain.
- In a second step, we use the results of the first to obtain an expression for the joint probability model—a so-called lower expectation operator on the sample space of possible paths—of an imprecise continuous-time Markov chain that is amenable to further exploration **(Work Package 1b)**. We also investigate whether this lower expectation operator can be expressed as a lower envelope of

expectation operators associated with more traditional, measure-theoretic stochastic processes.

- The final step consists in studying the mathematical properties of the continuous-time imprecise Markov model **(Work Package 1c)**. As a first special case, we intend to check whether it allows for a derivation from first principles of a non-linear variant of the Chapman–Kolmogorov equations, similar to what Škulj [22] found using more *ad hoc* arguments. That something similar is possible—and fairly straightforward—in the discrete-time case [9], should serve as an indication that this is indeed feasible. A second special case will be to define stopping times, and to study their basic properties.

Since the Chapman-Kolmogorov equations and stopping times lie at the basis of many computational methods for (precise) continuous-time Markov chains, we expect Work Package 1c to yield results that are useful to advance the second—computational—line of research that we are about to introduce (especially Work Package 2b). In order to take advantage of this overlap, we will provide the respective researchers with the opportunity to collaborate on these topics.

Computational methods **(Research Line 2)**.

While precise Markov chain theory often relies heavily on linear algebra, this is no longer true for imprecise Markov chains, where we need to resort to linear programming techniques. Consequently, in the majority of cases, solutions will have to be obtained in numerical form. Computational methods are therefore important, and must be developed alongside with theoretical concepts. The second general goal of this project is therefore to develop and improve numerical methods. This line of research can be divided into the following four work packages.

- The first step will be to define and compute coefficients of ergodicity (and other contraction measures) for imprecise continuous-time Markov chains **(Work Package 2a)**. By analogy with the discrete-time case [25], we expect it will be difficult to evaluate the theoretical definitions directly, so indirect computational methods will need to be developed. To do so, we will need to be able to efficiently compute distances between coherent lower previsions that are only partially specified. Known numerical examples suggest that this problem is challenging but solvable.
- The next task **(Work Package 2b)** is to develop methods for calculating tight bounds on expectations of functions of the states of an imprecise Markov chain. First, we intend to extend existing methods for functions that depend on the state at a single time in the future [22], which fail when the time interval grows large. To overcome this, we intend to exploit the contracting nature of Markov transition operators, using the coefficients of ergodicity of Work Package 2a. Later, we will also try and compute expectations for more general functions, including important stopping times—the expected time to absorption and expected return times—and probabilities of general events—absorption probabilities.
- The third task **(Work Package 2c)** is error estimation. Regardless of the method used, numerical errors seem inevitable in continuous-time models, where only a finite number of optimisation steps are feasible, whereas in theory, an optimisation would actually be needed in each intermediate time point. This gives rise to numerical errors, which are in every step transferred to the next steps as perturbations. Existing error estimates work well for short time intervals, but tend to significantly overestimate the errors for larger time intervals, as has been observed experimentally in simple problems.
- An important part of the error estimation will be a perturbation analysis, which is also of independent interest and will therefore be explored as a separate research task **(Work Package 2d)**. We will analyse how perturbations of its parameters affect the distance between an imprecise continuous-time Markov chain and its perturbed version. Such a perturbation analysis has been successfully applied

to imprecise discrete-time Markov chains; we expect it to be equally successful in continuous time.

As discussed, this computation-oriented research will benefit from the theoretical results in Research Line 1, and the respective researchers will be expected to collaborate. Similarly, the computational methods that we develop here (Work Package 2b and 2c) will benefit the study of limit distributions that we intend to conduct for Research Line 3 (Work Package 3b), because this study will involve computing limit distributions numerically; here too, the respective researchers will be expected to collaborate.

Limit behaviour and stationary distributions **(Research Line 3)**.

Limit behaviour is a crucial topic in Markov chain theory, and if a unique stationary distribution exists, it is often a central object of interest. In the precise case, linear algebra provides powerful tools for the analysis of limit behaviour, but no such methods are available for imprecise Markov chains. For imprecise discrete-time Markov chains, alternative methods have been developed [9], but in continuous time, little is known. Therefore, our third main goal is to study and characterise the limit behaviour of imprecise continuous-time Markov chains. This line of research can be divided into three work packages:

- The first task will be to find out under which conditions an imprecise continuous-time Markov chain converges to a limit distribution **(Work Package 3a)**. When such a limit distribution exists, we will also characterise the conditions under which it depends on the initial state of the chain and the conditions under which it is stationary. In discrete time, such a study has already been conducted successfully [9, 11]. In continuous time however, we are only aware of some partial answers [4].
- Once we have established the existence of a limit distribution, the next task will be to develop methods that allow us to compute it **(Work Package 3b)**. In the precise case, this is relatively easy, as it requires solving a linear system of equations. In the imprecise case, this system becomes non-linear, and solving it is far more difficult. We envision two approaches. The first option is to try and solve this system directly. We expect this to be feasible only in special cases. Whenever it is not, we will resort to the second option, which is to compute the limit distribution more naively: to actually approach the limit up to some desired accuracy. Since this second option will clearly benefit from the results in Work Packages 2b and 2c, we intend for the respective researchers to collaborate on these topics.
- A third task will be to analyse the structure of limit distributions: the types of classes the states belong to **(Work Package 3c)**. We expect this to be challenging because, due to their generality, imprecise continuous-time Markov chains will allow for a far richer range of classes of states and transitions between them than in the precise case. Our aim is to investigate the induced accessibility relations and their influence on convergence, especially when it is not unique, and to characterise and classify the invariant distributions. As a first step, we will extend the methodology in [21]—a partial classification of invariant sets for discrete-time imprecise Markov chains—to continuous time.

Contingency plans **(Work Packages 4 & 5)**.

Although we expect to finish each work package, we might of course run into problems: some computations might be inherently intractable, or there might be theoretical questions we are unable to answer. Even so, this would not endanger the aim of our project: to make significant progress in the field of continuous-time Markov chains. Indeed, since this field is still essentially wide open, and because both project partners have been instrumental in developing the discrete-time version, it should not be a problem to make significant progress in each of the three proposed research lines. Nevertheless, should we need to absorb major setbacks, the following additional research topics can serve as contingency plans.

They also serve as extra topics should the intended research proceed faster than expected.

First, as is clear from the discussion above, the proposed research does not work towards a specific application, nor does it try to build an ad-hoc model for some specific problem. Rather, the aim is to develop a general theory of continuous-time Markov chains. Nevertheless, our results can be used to study and solve a variety of practical problems. Since real applications are an ideal testing ground for new theory, it would be nice to tackle such applications **(Work Package 4)**; the choice of application will depend on the level of complexity that the developed framework will by then be able to deal with.

A second extra research topic is time reversibility. This concept is very important for (precise) stochastic processes, but it has not yet been systematically studied in the framework of imprecision; to the best of our knowledge, the preliminary results in Reference [24] are the only exception. Therefore, a systematic analysis of imprecise continuous-time reversible Markov chains **(Work Package 5)** would definitely be an interesting research topic to pursue.

Provide a work plan, i.e. the different work packages and detailed timetable.
Describe the different work packages (WP) the proposed research work will be divided in. Indicate for each WP the time that it is expected to take. You might use a table or another type of scheme to clarify the work plan. Clearly indicate the contribution of each project partner, taking into account the complementary expertise of the project partners.

	Short description	**1st year**				**2nd year**				**3rd year**				**4th year**			
	Joint models and properties																
WP1a	Probability tree model	G	G	G	G	G											
WP1b	Expressions for the joint				G	G	G	G	G	G							
WP1c	Mathematical properties						G	G	G	B	B	B	B	B	B		
	Computational methods																
WP2a	Coefficients of ergodicity	L	L	L	L	B	B	B	B								
WP2b	Compute thight bounds							L	L	B	B	B	B	B	B		
WP2c	Error estimation									L	L	B	B	B	B		
WP2d	Perturbation analysis				L	L	L	L	L	L							
	Limit behaviour																
WP3a	Existence of limit distributions	G	G	G	G	B	B	B	B								
WP3b	Compute limit distributions									G	G	B	B	B	B		
WP3c	Characterise limit distributions					G	G	G	G	B	B	B	B				
	Contingency plans																
WP4	Applications							B	B	B	B	B	B	B	B		
WP5	Time reversal							L	L	L	L	B	B	B	B		

At the universities of Ghent and Ljubljana, a PhD fellowship, and therefore also the work on the proposed research, is usually spread over a period of four years. We have indicated these four years in the table above, and have divided every year into four periods of three months (i.e. quarters). The work on the research has already been divided in work packages in the previous section. For each work package, the table provides a short description and indicates the quarters during which we expect the researchers to be working on it.

We mark a box with a G to indicate that the research on that topic, in that specific quarter, will be led by the Ghent group; an L indicates that the research will be led by the Ljubljana group. For some of the work packages, after the initial research on that topic has been carried out, we plan to visit each other to discuss the results, followed by joint work to finalise that part of the research; we indicate this in the table by marking the corresponding box with a B (which stands for 'both'). As explained in the methodology section, this collaboration is essential for work packages WP1c, WP2b, WP2c and WP3b, because we expect the results that are obtained in these work packages to benefit from each other. For work packages WP2a, WP3a, WP3c, WP4 and WP5, the planned collaboration is not essential, but nevertheless recommended because both partners have a mutual interest and expertise in these topics. After the work on a specific work package is finished, the results will be disseminated at research conferences and published in scientific journals. The last two quarters of the fourth year are intentionally left blank, because these will be reserved for writing the PhD theses.

Enumerate the bibliographical references that are relevant for your research proposal.

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Indicate below whether you think the results of the proposed research will be suitable to be communicated to a non expert audience and how you would undertake such communication.
FWO encourages its fellows to disseminate the results of their research widely, and valorize them where possible.

Markov chains are definitely suitable for communication to a non-expert audience. Their basics are easy to explain to an audience with limited maths. Also, they can be used to describe many practical problems, ranging from basic strategies for playing certain games to demographic predictions, planning of workforce recruitment and promotion strategies. For example, UGhent research on queueing theory—which uses Markov chains extensively—has recently been cleverly applied to waiting in line at a festival bar, and its findings were easily picked up by several national media. The addition of imprecision to such problems only increases their potential for communication to a non expert audience, because it allows us to include aspects such as safety, reliability and robustness, all of which are highly relevant to society.

In addition to purely educative or demonstrative purposes, Markov chains can also be used to develop relatively simple web-based tools that can serve to support business processes. The Slovenian group has been involved in the successful development of such a web-based platform for prediction and strategy testing for the structure of Slovenian armed forces. Such platforms would definitely benefit from models that allow for imprecision as well.