Modeling with Markov chains: The MARMOTE Software

Labex UCN seminar

Sophia Antipolis 3 september 2015

1 Markov modeling

Markov modeling

What is a Markov Chain
What is a Markov modeler

Markov chains

Markov chains/processes are a class of stochastic processes $X(t)$, $t \in \mathbb{Z}$ or $\mathbb{R}$

- evolving on a state space $\mathcal{E}$
- described by a transition rule

$$i \longrightarrow j \quad \text{with probability } p_{ij}$$

$$i \longrightarrow j \quad \text{with rate } \lambda_{ij}$$

- from some initial state

Markov chains, ctd

Many properties of Markov chains can be obtained

- by analyzing the graph of transitions
- by solving problems of linear algebra

Markov modeling

Markov modeling consists in

- constructing Markov models
- analyzing them:
  - determine qualitive properties: structure, ergodicity, stability ...
  - compute metrics related with probabilities, frequencies, times, durations ...

Two main "profiles" + mixed ones

Markov modelers, type 1

Theoretician: Aims at developing MC solution methods

- as generic as possible
- yet taking into account the structure of the model

Involves:

- invent new formulas/algorithms
- program new methods
- test them on examples/benchmarks
- compare with previous methods (exec. time, accuracy)

Markov modelers, type 2

Practician: Develops Markov models for specific applications
Involves:

- describe/represent model (parameters, structure, ...)
- test model with simulation
- solve model (analytic, numerical), loop until model passes tests
- execute experimental plans
- compare different models (e.g. simplifications)

The MARMOTE project

MARMOTE: MARkovian MOdeling Tools and Environments
ANR-12-MONU-0019
2013 – 2016

Objectives:

- Develop Markov Enviromnent
- New solution and simulation techniques
- Application test-cases

MARMOTE Software

Objectives of the MARMOTE Software platform:

Initial specifications

To provide to the general scientist a "modeling environment" which must give access to algorithms developed by specialists. Principal characteristics: be as open as possible, be component-oriented, contributive. Will be populated with a modeling language, a minimal user interface, minimal solution algorithms.

MARMOTE Software base

Secondary objective: unify existing software

The partners bring existing software packages

- Psi, Psi2, Psi3 (Perfect Simulation, INRIA/MESCAL)
- Xborne (Solutions with bounds for MC-related distributions, UVSQ/PRiSM)
- ERS (Basic MC solution)

Other software around

- PEPS
- GreatSPN
- Tangram II
- ...

Requirements

Modeling abstraction

- possibility to handle formal models, infinite state spaces, ...

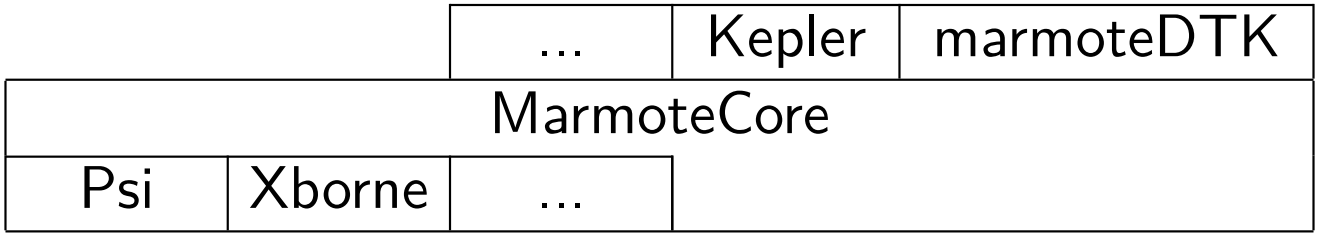
Other requirements came along the way:

- possibility to communicate with other modeling/solution systems: matlab, R, ...
- possibility to be used in workflow management systems
- possibility to implement multiple solution methods for different types of Markov chains

Architecture

Target Architecture in three layers:

- Bottom: solution methods
- Middle: Marmote API, construction of models, handling of data, algorithms, results
- Top: GUI and workflow management



Choice of an object-oriented language: C++

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The MARMOTE Core

Main Objects

Classes currently implemented

- Markov chains: `markovChain` and derived classes
- Transitions: `transitionStructure`
- State Spaces: `marmoteSet`
- `Distribution` and derived classes

The Distribution object

Methods

```
virtual double mean() = 0;
virtual double rate() = 0; // inverse of the mean
virtual double moment(int n) = 0;
double variance();
virtual double laplace(double s) = 0;
virtual double dLaplace(double s) = 0;
virtual double cdf(double x) = 0;
double ccdf(double x)  return 1.0 - cdf(x); ;
virtual bool hasMoment(int n) = 0;
virtual Distribution* rescale(double factor) = 0;
virtual Distribution* copy() = 0;
virtual double sample() = 0;
virtual void iidSample(int n, double* s) = 0;
virtual double distanceL1(Distribution*);
virtual bool hasProperty(std::string);
```

Distributions

Distributions implemented:

- `Distribution/discreteDistribution`
  - `Distribution/diracDistribution`
  - `Distribution/bernoulliDistribution`
  - `Distribution/uniformDiscreteDistribution`
  - `Distribution/geometricDistribution`
- `Distribution/exponentialDistribution`
- `Distribution/uniformDistribution`

Transition Structures

Methods

```
timeType getType()  return _type; ;
virtual double getEntry(int,int) = 0;
virtual int getNbElts(int) = 0;
virtual int getCol(int,int) = 0;
virtual double getEntryByCol(int,int) = 0;
virtual DiscreteDistribution* getTransDistrib(int) = 0;
// transitions from some state and their probas
bool readEntry(FILE*);
virtual double rowSum(int) = 0;
virtual transitionStructure* uniformize() = 0;
virtual void evaluateMeasure(double*,double*);
virtual void
evaluateMeasure(DiscreteDistribution*,DiscreteDistribution*);
virtual void evaluateValue(double*,double*) = 0;
```

Transition structures

Transition structures implemented:

- `transitionStructure/sparseMatrix`
- `transitionStructure/multiDimHomTransition` (generalized birth-death)
- `transitionStructure/eventMixture`

Projected:

- `transitionStructure/matrix`
- `transitionStructure/QBD`

State spaces

Attributes of marmoteSet

```
enum opType  UNION, PRODUCT, SIMPLE ;
bool _isSimple, _isUnion, _isProduct;
int _nbDimensions;
int _nbZones;
long int _cardinal;
marmoteSet** _zone;
marmoteSet** _dimension;
int* _stateBuffer;
int* _dimOffset;
int* _idxOffset;
int _totNbDims;
int* _zeroState;
```

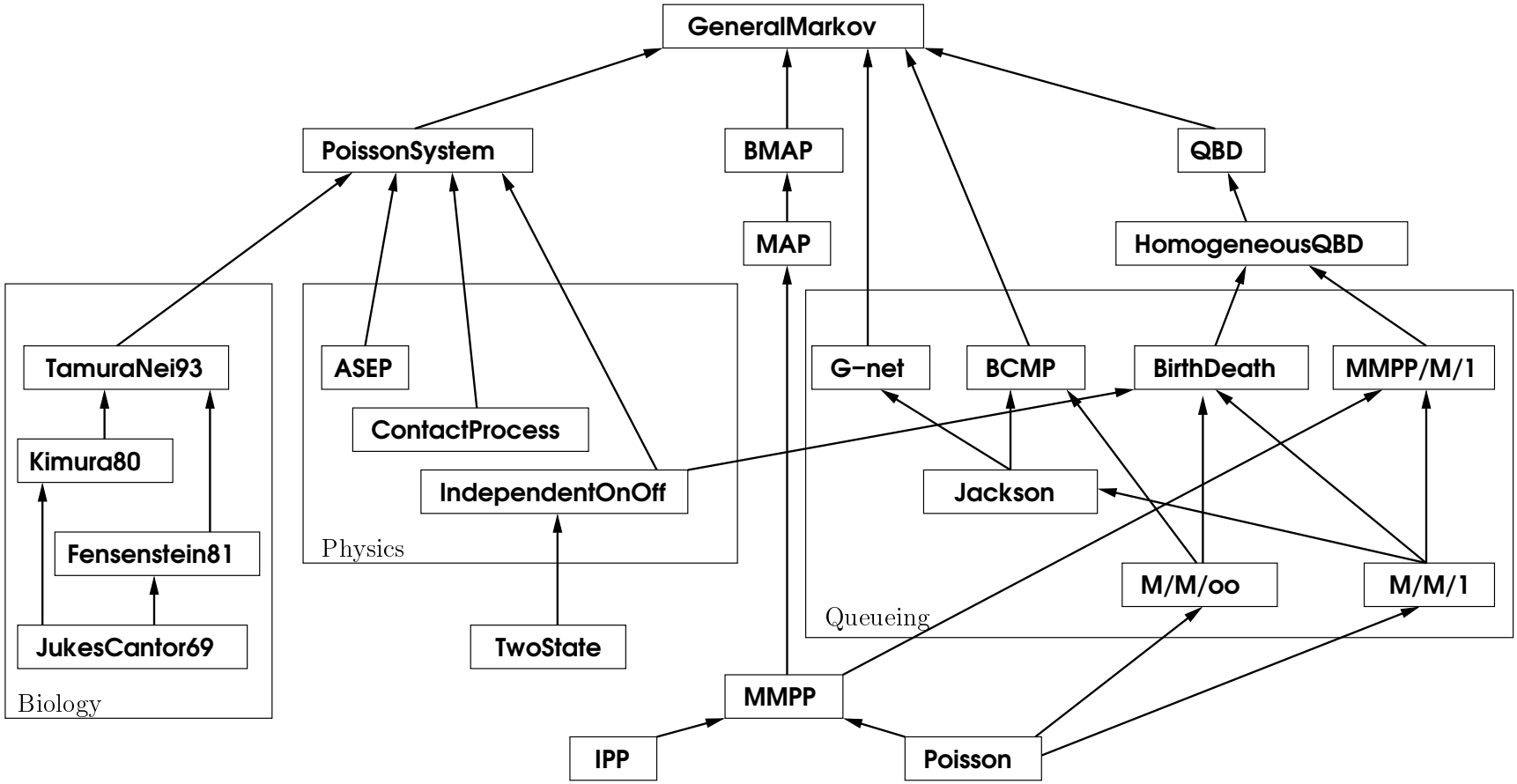
Marmote sets, ctd

Methods

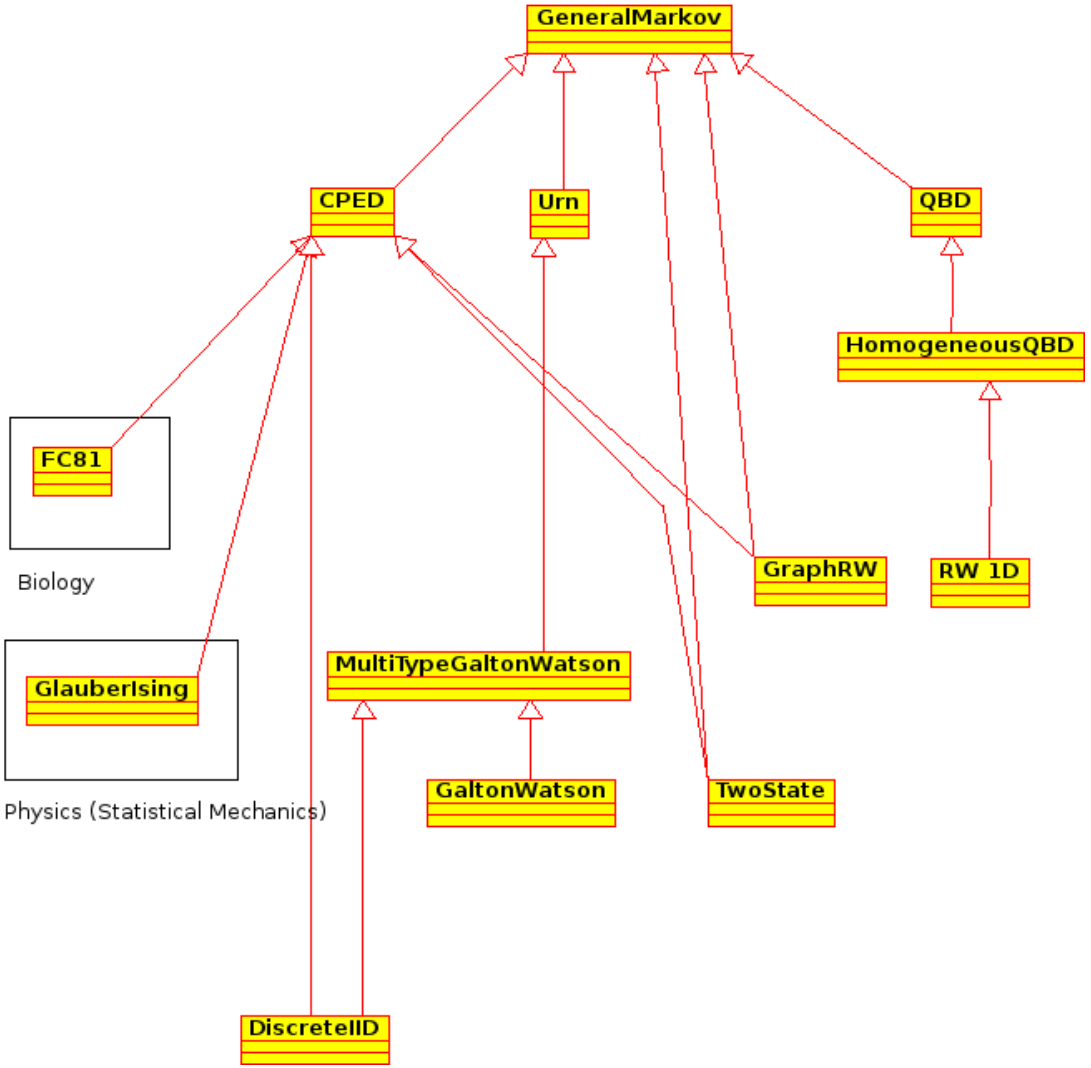
```
// constructors
marmoteSet();
marmoteSet( marmoteSet **list, int nb, opType t );
// accessors
virtual long int cardinal();
bool isFinite(), bool isSimple(), bool isUnion(), bool
isProduct();
int totNbDims();
// state-index conversions
virtual void decodeState(int index, int* buffer);
int index(int* buffer);
// state space exploration
virtual void firstState(int* buffer);
virtual void nextState(int* buffer);
virtual bool isZero(int* buffer);
// utilities
virtual void enumerate();
virtual void printState(FILE* out, int index);
```

3 The Markov chains

Markov Zoo


GeneralMarkov
PoissonSystem
BMAP
QBD
MAP
HomogeneousQBD
TamuraNei93
ASEP
G−net
BCMP
BirthDeath
MMPP/M/1
ContactProcess
Kimura80
IndependentOnOff
Jackson
Physics
Fensenstein81
M/M/oo
M/M/1
Queueing
JukesCantor69
TwoState
MMPP
Biology
IPP
Poisson

Markov Zoo


GeneralMarkov
CPED
Urn
QBD
HomogeneousQBD
FC81
Biology
GraphRW
RW 1D
GlauberIsing
MultiTypeGaltonWatson
Physics (Statistical Mechanics)
GaltonWatson
TwoState
DiscreteIID

The Markov Chain object

Principles:

- "concrete" chains
  - read/create from files in several formats Ers, Marca...
    $\Longrightarrow$ being implemented: HBF, Xborne transition spec, PSI spec
  - create from a `transitionStructure` (e.g. matrix)
  - write to file in Ers format
    $\Longrightarrow$ being implemented: Marca, HBF, R, scilab/matlab, Maple, ...
- "virtual" chains specified by
  - format
  - name of model
  - optional liste of extensions and/or file names

"lazy" evaluation

Attributes

Attributes of MarkovChain

```
timeType _type;
int _stateSpaceSize;
transitionStructure* _generator;
DiscreteDistribution* _initDistribution;

// fields related to abstractness and file names
bool _isAbstract;
int _abstractNbre;
string* _abstract;
string _format;
string _modelName;
```

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Programming Markov Chains

Creation

Three classes of possibilities:

1. read the generator (and the state space) in a file
2. use a predefined class
3. create the generator “by hand”

Creation/Read

Creation code

```
markovChain* c4 = new markovChain( "Xborne", NULL, 0, "rw1d", true );
markovChain* c5 = new markovChain( "PSI", NULL, 0, "rw1d", true );
markovChain* c6 = new markovCHain( "Ers", NULL, 0, "rw1d", false );
```

Virtual chains:

$\Longrightarrow$ formats PSI1/MARCA, ERS, Xborne/C, Xborne/Rii

Concrete chains:

$\Longrightarrow$ formats ERS, MARCA

Interface read

```
/**
* @brief Constructor for Markov chains from files in various formats.
* In the abstract form:  just stores the name(s) of the files that
* define the mode.  In the non-abstract (concrete) form:  the chain is
* instantiated in the memory with a concrete transition structure.
* @param format the format or language in which the model is specified
* @param param[] is the list of parameters
* @param nbreParam the size of param
* @param modelName name of the model, usually the prefix of various
files
* @param isAbstract specifies if the chain is abstract or not
* @return Markov Chain
*/
markovChain(string format, string param[], int nbreParam,
            string modelName, bool isAbstract);
```

Creation/Use

Direct use of one of the pre-programmed classes.
Currently implemented: small part of the Markov Zoo

- felsenstein81, a model for BioInformatics
- homogeneous1DRandomWalk
- homogeneousMultiDRandomWalk
- homogeneous1DBirthDeath
- ...

Creation/Make

Typically in two steps:

1. create a `transitionStructure` object
2. create the Markov chain from this object

Ecample of creation code

```
sparseMatrix* gen = makeGenerator( sp, N, E1, E2, M, nu );
markovChain* myMC = new markovChain( gen );
```

Creation with a state space

Objects of type `marmoteSet` are useful to create the generator:

```
sparseMatrix* makeGenerator(layeredStateSpace* sp, ...  )  {

  sparseMatrix* gen = new sparseMatrix( sp->cardinal() );

  int stateBuffer[5];
  sp->firstState(stateBuffer);
  int idx = 0;
  do {
    ...
    // destination state stored in nextBuffer
    nextBuffer[0] = MIN( stateBuffer[0] + 1, someBound );
    ...
    gen->addToEntry( idx, sp->index(nextBuffer), someRate );
    gen->addToEntry( idx, idx, -someRate );
    ...

    sp->nextState( stateBuffer );
    idx++;
  } while (!sp->isZero(stateBuffer));
}
```

5 Computing with Markov Chains

Available Solution Methods for `MarkovChain`

Monte Carlo Simulation (forward)

```
virtual simulationResult* simulateChain(double, bool, bool, bool, bool);
virtual simulationResult* simulateChainDT(int, bool, bool, bool);
virtual simulationResult* simulateChainCT(double, bool, bool, bool,
bool);
 simulationResult* simulatePSI(int, bool, bool, bool);
```

Exact sampling from the stationary distribution (backwards)

```
simulationResult* stationaryDistributionSample (int nbSamples);
```

Solution methods, ctd

Computation of the stationary distribution

```
virtual Distribution* stationaryDistribution(bool);
virtual Distribution* stationaryDistributionCT(bool);
virtual Distribution* stationaryDistributionDT(bool);
Distribution* stationaryDistributionGhtLD();
Distribution* stationaryDistributionSOR();
```

Entry point

```
Distribution* stationaryDistribution_iterative(
                string method,
                int tmax,
                double precision,
                string initDistribType,
                discreteDistribution* initDistrib,
                bool progress );
```

Ctd.

Hitting times

```
Distribution * hittingTimeDistribution (int iState, bool
*hitSetIndicator);
int * simulateHittingTime (int iState, bool *hittingSet, int nbSamples,
int tMax);
double* averageHittingTime (bool *hitSetIndicator);
double* averageHittingTimeDT (bool *hitSetIndicator);
double* averageHittingTimeDT_iterative (bool *hitSetIndicator);
```

Simulations

Simulating uses a variety of parameters and provides a variety of results → specific object `simulationResult`

Attributes

```
timeType _type;
int _stateSpaceSize;
int _trajectorySize;
bool _hasDistrib;
bool _hasTrajectory;
DiscreteDistribution* _distrib;
double* _dates;
double* _increments;
int* _states;
```

Methods

```
simulationResult(int size, timeType t, bool stats);
simulationResult(string format, string modelName, bool stats);
```

Utilities for MarkovChain

Utilities

```
virtual MarkovChain* copy();
virtual MarkovChain* uniformize();
virtual MarkovChain* embed();
void write( string format );
```

Other

Direct solution methods for specific chains:

- `homogeneous1DRandomWalk`

```
DiscreteDistribution* transientDistribution(int t, int nMax);
GeometricDistribution* stationaryDistribution();
DiscreteDistribution* stationaryDistribution(int nMax);
simulationResult* simulateChain(long int tMax, bool stat, bool
traj, bool trace);
```

- `felsenstein81`

```
DiscreteDistribution* transientDistribution(double);
DiscreteDistribution* stationaryDistribution();
simulationResult* simulateChain(double, bool stat, bool traj,
bool incr, bool trace);
```

Further code examples

Comparison of computations for the stationary distribution

```
// specific methods for F81
felsenstein81* c1 = new felsenstein81(...);
Distribution* d1 = c1->stationaryDistribution();
Distribution* d2 = c1->simulateChain(...)->getDistribution();
// generic methods for MCs
MarkovChain* c2 = static_cast<MarkovChain*>(c1);
Distribution* d3 = c2->stationaryDistribution_GaussSeidel();
Distribution* d4 = c2->stationaryDistribution_PowerMethod();
Distribution* d5 = c2->stationaryDistribution_Xborne_LowBound();
Distribution* d6 = c2->replicateSamples_Psi3(...);
Distribution* d7 = c2->simulateChain(...)->getDistribution();
Distribution* d8 = c2->simulateChain2(...)->getDistribution();
// comparison
cout << "Distance L1(d1,d2) = " << d1->distanceL1(d2) « endl;
```

6 Conclusion

As a conclusion

An ongoing development

- interfaces with R
- addition of solution methods
- more interface formats
- ...

An open development

- in need of users/testers
- in need of contributers