Evaluating dependability metrics of critical systems: Monte Carlo techniques for rare event analysis

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# Part I

#### Introduction

- 2 Monte Carlo: the basics
- Inefficiency of crude Monte Carlo, and robustness issue
  - Importance Sampling
- 5 Splitting
- 6 Confidence interval issues

(Part II is devoted to representative applications)

# Outline

### Introduction

- 2 Monte Carlo: the basics
- Inefficiency of crude Monte Carlo, and robustness issue
- Importance Sampling

#### 5 Splitting

6 Confidence interval issues

# Simulation

- Simulation here means discrete event simulation.
- No difference will be done with Monte Carlo in this tutorial.
- Standard background:
  - simulation in general,
  - transient measures analysis using simulation,
  - equilibrium measures analysis using simulation, and its main problems:
    - eliminating the transient phase,
    - ★ stopping the simulation process.
- Main problems in dependability:
  - building (specifying) models,
  - handling rare events;
  - the tutorial is structured around this last problem.

#### Rare events

Rare events occur when dealing with performance evaluation in many different areas

- in *telecommunication networks*: loss probability of a small unit of information (a packet, or a cell in ATM networks), connectivity of a set of nodes,
- in *dependability analysis*: probability that a system is failed at a given time, availability, mean-time-to-failure,
- in air control systems: probability of collision of two aircrafts,
- in particle transport: probability of penetration of a nuclear shield,
- in *biology*: probability of some molecular reactions,
- in insurance: probability of ruin of a company,
- in *finance*: value at risk (maximal loss with a given probability in a predefined time),
- ...

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## What is a rare event? Why simulation?

- A rare event is an event occurring with a small probability.
- How small? Depends on the context.
- In many cases, these probabilities can be between  $10^{-8}$  and  $10^{-10}$ , or even at lower values. Main example: critical systems, that is,
  - systems where the rare event is a catastrophic failure with possible human losses,
  - or systems where the rare event is a catastrophic failure with possible monetary losses.
- In most of the above problems, the mathematical model is often too complicated to be solved by analytic or numeric methods because
  - the assumptions are not stringent enough,
  - the mathematical dimension of the problem is too large,
  - the state space is too large to get a result in reasonable time,
  - ► ...
- Simulation is, most of the time, the only tool at hand.

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## Rare events in dependability

- System's failure usually is (should be) a rare event.
- This translates into:
  - reliability at  $t \approx 1$
  - Mean Time To Failure  $\gg 1$
  - availability at  $t \approx 1$
  - ▶ interval availability on [0, t] has a distribution close to a Dirac at 1
  - etc.
- This explains why in dependability, standard simulation techniques are often hard or impossible to use.

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# Monte Carlo

- In all the above problems, the goal is to compute μ = E[X] for some random variable X (that is, it can be written in this form).
- Monte Carlo simulation (in its basic form) generates n independent copies of X, (X<sub>i</sub>, 1 ≤ i ≤ n). Then,
  - $\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i$  is an approximation (an estimation) of  $\mu$ ;
  - $\bar{X}_n \to \mu$  with probability 1, as  $n \to \infty$  (Strong Law of Large Numbers).

• Accuracy: how accurate is  $\bar{X}_n$ ? We can evaluate the accuracy of  $\bar{X}_n$  by means of the Central Limit Theorem, which allows us to build the following confidence interval:

$$CI = \left(\bar{X}_n - \frac{c_\alpha \sigma}{\sqrt{n}}, \, \bar{X}_n + \frac{c_\alpha \sigma}{\sqrt{n}}\right)$$

- meaning:  $\mathbb{P}(\mu \in CI) \approx 1 \alpha$ ;  $\alpha$ : confidence level
- (that is, on a large number M of experiences (of estimations of  $\mu$  using  $\overline{X}_n$ ), we expect that in roughly a fraction  $\alpha$  of the cases (in about  $\alpha M$  cases), the confidence interval doesn't contain  $\mu$ )
- $c_{\alpha} = \Phi^{-1}(1 \alpha/2)$  where  $\Phi$  is the cdf of  $\mathcal{N}(0, 1)$
- $\sigma^2 = \operatorname{Var}[X] = \mathbb{E}[X^2] \mathbb{E}^2[X]$ , usually unknown and estimated by

$$S_n^2 = \frac{1}{n-1} \sum_{i=1}^n X_i^2 - \frac{n}{n-1} \bar{X}_n^2.$$

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## Remarks on the confidence interval

- Size of the confidence interval:  $2c_{\alpha}\sigma/\sqrt{n}$ .
- The smaller  $\alpha$ , the more confident we are in the result:

 $\mathbb{P}(\mu \text{ belongs to } CI) \approx 1 - \alpha.$ 

• But, if we reduce  $\alpha$  (without changing *n*),  $c_{\alpha}$  increases:

• 
$$\alpha = 10\%$$
 gives  $c_{\alpha} = 1.64$ ,

• 
$$\alpha = 5\%$$
 gives  $c_{\alpha} = 1.96$ 

• 
$$\alpha = 1\%$$
 gives  $c_{\alpha} = 2.58$ 

- The other way to have a better confidence interval is to increase *n*.
- The 1/\sqrt{n} factor says that to reduce the width of the confidence interval by 2, we need 4 times more replications.

# A fundamental example: evaluating integrals

• Assume 
$$\mu = \int_{I} f(x) dx < \infty$$
, with I an interval in  $\mathbb{R}^{d}$ .

- With an appropriate change of variable, we can assume that  $I = [0, 1]^d$ .
- There are many numerical methods available for approximating μ. Their quality is captured by their *convergence speed* as a function of the number of calls to f, which we denote by n. Some examples:
  - Trapezium rule; convergence speed is in  $n^{-2/d}$ ,
  - Simpson's rule; convergence speed is in  $n^{-4/d}$ ,
  - Gaussian quadrature method having *m* points; convergence speed is in  $n^{-(2m-1)/d}$ .

For all these methods, the speed decreases when d increases (and  $\rightarrow 0$  when  $d \rightarrow \infty$ ).

## The "independence of the dimension"

- Let now U be an uniform r.v. on the cube  $[0,1]^d$  and X = f(U).
- We immediately have μ = E(X), which opens the path to the Monte Carlo technique for approximating μ statistically.
- We have that
  - $\bar{X}_n$  is an estimator of our integral,
  - ► and that the convergence speed, as a function of n, is in n<sup>-1/2</sup>, thus independent of the dimension d of the problem.
- This independence of the dimension of the problem in the computational cost is the main advantage of the Monte Carlo approach over quadrature techniques.
- In many cases, it means that quadrature techniques can not be applied, and that Monte Carlo works in reasonable time with good accuracy.

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## Other examples

- Reliability at t:
  - C(t) is the configuration of a multicomponent system at time t;
  - s(c) = 1 (when configuration is c, system is operational)

• 
$$X(t) = 1(s(C(u))) = 1$$
 for all  $u \le t$ )

- $\bar{X}_n(t) = n^{-1} \sum_{i=1}^n X_i(t)$  is an estimator of the reliability at t, with  $X_1(t), \dots, X_n(t)$  n iid copies of X(t)
- Mean waiting time in equilibrium:
  - ► X<sub>i</sub> is the waiting time of the *i*th customer arriving to a stationary queue,
  - $\bar{X}_n$  is an estimator of the mean waiting time in equilibrium.

etc.

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## Improving Monte Carlo methods

- Given a problem (that is, given X), there are possibly many estimators for approximating  $\mu = \mathbb{E}(X)$ .
- For any such estimator  $\widetilde{X}$ , we can usually write

$$\widetilde{X}=\phi(X_1,\cdots,X_n)$$

where  $X_1, \dots, X_n$  are *n* copies of *X*, not necessarily independent in the general case.

- How to compare X with the standard X? Or how to compare two possible estimators of μ, X<sub>1</sub> and X<sub>2</sub>?
- Which good property for a new estimator  $\widetilde{X}$  must we look for?
- A first example is unbiasedness:  $\widetilde{X}$  is unbiased if  $\mathbb{E}(\widetilde{X}) = \mu$ , which obviously looks as a desirable property.
- Note that there are many useful estimators that are not unbiased.

- From the accuracy point of view, the smallest the variability of an unbiased estimator (the smallest its variance), the better its accuracy.
- For instance, in the case of the standard estimator  $\bar{X}$ , we have seen that its accuracy is captured by the size of the associated confidence interval,  $2c_{\alpha}\sigma/\sqrt{n}$ .
- Now observe that this confidence interval size can be also written  $2c_{\alpha}\sqrt{\mathbb{V}(\bar{X})}$ .
- A great amount of effort has been done in the research community looking for new estimators of the same target  $\mu$  having smaller and smaller variances.
- Another possibility (less explored so far) is to reduce the computational cost.
- Let's look at this in some detail, focusing on the variance problem.

- Before looking at some ideas developed to build estimators with "small" variances, let us look more formally at the accuracy concept.
- The variability of an estimator  $\widetilde{X}_n$  of  $\mu$  is formally captured by the Mean Squared Error

$$\mathsf{MSE}(\widetilde{X}_n) = \mathbb{E}[(\widetilde{X} - \mu)^2], = \mathbb{V}(\widetilde{X}_n) + \mathbb{B}^2(\widetilde{X}_n),$$

where  $\mathbb{B}(\widetilde{X}_n)$  is the Biais of  $\widetilde{X}_n$ ,

$$\mathbb{B}(\widetilde{X}_n) = \big| \mathbb{E}(\widetilde{X}_n) - \mu \big|.$$

- Recall that many estimators are *unbiased*, meaning that  $\mathbb{E}(\widetilde{X}_n) = \mu$ , that is,  $\mathbb{B}(\widetilde{X}_n) = 0$  (and then, that  $MSE(\widetilde{X}_n) = \mathbb{V}(\widetilde{X}_n)$ ).
- In any case, the dominant term is always the variance one.
- In the following refresher, the goal is to estimate μ = E(X) where X has cdf F and variance σ<sup>2</sup>. Recall that V(X
  <sub>n</sub>) = σ<sup>2</sup>/n.

### Variance reduction: antithetic variables

- Suppose *n* is even, that is, n = 2k.
- Assume that the *i*th replication  $X_i$  is obtained using  $X_i = F^{-1}(U_i)$ , with  $U_1, \dots, U_n$  i.i.d. with the Uniform(0,1) distribution.
- Let us define a new estimator X
  <sub>2k</sub> using half the previous number of uniform r.v.: X
  <sub>2k</sub> is built from U<sub>1</sub>,..., U<sub>k</sub> using

$$\widetilde{X}_{2k} = \frac{1}{2k} \sum_{j=1}^{k} \Big[ F^{-1}(U_j) + F^{-1}(1 - U_j) \Big].$$

 Observe that if U is Uniform(0,1), 1 – U has the same distribution and both variables are negatively correlated:

$$\mathbb{C}\mathsf{ov}(U, 1-U) = \mathbb{E}[U(1-U)] - \mathbb{E}(U)\mathbb{E}(1-U) = -1/12$$

• For the variance of  $\widetilde{X}_{2k}$ ,

$$\mathbb{V}(\widetilde{X}_{2k}) = \frac{1}{4k^2} \sum_{j=1}^k \mathbb{V}(Y_j + Z_j),$$

with  $Y_j = F^{-1}(U_j)$  and  $Z_j = F^{-1}(1 - U_j)$ .

• After some algebra, writing back 2k = n,

$$\mathbb{V}(\widetilde{X}_n) = \frac{1}{n} \Big( \sigma^2 + \mathbb{C}\mathrm{ov}(Y, Z) \Big),$$

with (Y, Z) representing any generic pair  $(Y_j, Z_j)$ .

 It can now be proven that Cov(Y, Z) ≤ 0, due to the fact that F<sup>-1</sup> is not decreasing and that U and 1 – U are negatively correlated, and thus

$$\mathbb{V}(\widetilde{X}_n) \leq \mathbb{V}(\overline{X}_n).$$

This technique is called antithetic variables in Monte Carlo theory.

### Variance reduction: common variables

- Suppose now that X is naturally sampled as X = Y Z, Y and Z being two r.v. defined on the same space, and dependent.
- Let us denote  $\mathbb{V}(Y) = \sigma_Y^2$ ,  $\mathbb{V}(Z) = \sigma_Z^2$ ,  $\mathbb{C}ov(Y, Z) = C_{Y, Z}$
- The standard estimator of µ is simply

$$\bar{X}_n = \bar{Y}_n - \bar{Z}_n.$$

Its variance is

$$\mathbb{V}(\bar{X}_n) = \frac{1}{n} \Big( \sigma_Y^2 + \sigma_Z^2 - 2C_{Y,Z} \Big).$$

To build Y
<sub>n</sub> and Z
<sub>n</sub> we typically use Y<sub>i</sub> = F<sub>Y</sub><sup>-1</sup>(U<sub>1,i</sub>) and Z<sub>j</sub> = F<sub>Z</sub><sup>-1</sup>(U<sub>2,j</sub>) where the U<sub>m,h</sub>, m = 1, 2, h = 1, · · · , n, are iid Uniform(0,1) r.v. and F<sub>Y</sub>, F<sub>Z</sub> are the respective cdf of Y and Z.

- Suppose now that we sample each pair  $(Y_k, Z_k)$  with the same uniform r.v.  $U_k$ :  $Y_k = F_Y^{-1}(U_k)$  and  $Z_k = F_Z^{-1}(U_k)$ .
- Using the fact that  $F_Y^{-1}$  and  $F_Z^{-1}$  are non increasing, we can easily prove that  $\mathbb{C}ov(Y_k, Z_k) \ge 0$ .
- This means that if we define a new estimator  $\widetilde{X}_n$  as

$$\widetilde{X}_n = \frac{1}{n} \sum_{k=1}^n \left[ F_Y^{-1}(U_k) - F_Z^{-1}(U_k) \right]$$

we have

$$\mathbb{E}(\widetilde{X}_n) = \mathbb{E}(\overline{X}_n) = \mu,$$

and

$$\mathbb{V}(\widetilde{X}_n) \leq \mathbb{V}(\overline{X}_n).$$

This technique is called common variables in Monte Carlo theory.

### Variance reduction: control variables

- Here, we suppose that there is an auxiliary r.v. C correlated with X, with known mean  $\mathbb{E}(C)$  and easy to sample.
- Define X̃ = X + γ(C − 𝔅(C)) for an arbitrary coefficient γ > 0. See that 𝔅(X̃) = μ.
- We have  $\mathbb{V}(\widetilde{X}) = \sigma^2 2\gamma \operatorname{Cov}(X, C) + \gamma^2 \mathbb{V}(C)$ .
- If Cov(X, C) and V(C) are known, we set γ = Cov(X, C)/V(C) and we get

$$\widetilde{X} = \left(1 - \varrho_{X,C}^2\right)\sigma^2 \le \sigma^2,$$

 $\rho_{X,C}$  being the coefficient of correlation between X and C.

## Variance reduction: conditional Monte Carlo

- Assume we have an auxiliary r.v. *C*, correlated with *X*, such that  $\mathbb{E}(X | C)$  is available analytically and *C* is easy to sample.
- Since E[E(X | C)] = μ, the r.v. E(X | C) is an unbiased estimator of μ.
- From

$$\sigma^2 = \mathbb{V}(X) = \mathbb{V}[\mathbb{E}(X \mid C)] + \mathbb{E}[\mathbb{V}(X \mid C)],$$

we get

$$\mathbb{V}[\mathbb{E}(X \mid C)] = \sigma^2 - \mathbb{E}[\mathbb{V}(X \mid C)] \le \sigma^2$$

because  $\mathbb{V}(X \mid C)$  and thus  $\mathbb{E}[\mathbb{V}(X \mid C)]$  are non negative.

• The corresponding estimator is

$$\widetilde{X}_n = \frac{1}{n} \sum_{i=1}^n \mathbb{E}(X \mid C_i).$$

## Monte Carlo drawbacks

- So, is there any problem with Monte Carlo approach?
- Main one: the rare event problem
- Second problem: specification/validation of (complex) models
- This tutorial focuses on the main one
- There are many techniques for facing the rare event problem:
  - for example, we have the variance reduction techniques described before (there are other similar methods available);
  - another possibility is to reduce the simulation time needed to get a replication
- This tutorial described the most important ones in dependability.

# Conclusions of Part I

- Dependability analysis of complex systems through simulation has two main problems:
  - computing small probabilities (or large averages),
  - and building/specifying/validating complex models.

Otherwise, simulation is (more or less) straightforward to apply.

- More formally, the problem with rare event is the lack of accuracy if we use standard Monte Carlo. The problem is so important that it often implies that standard simulation will simply not work.
- Concerning rare events, the most important method to allow Monte Carlo techniques to work is *importance sampling*. The second one in importance is called *splitting*.

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## What is crude simulation?

- Assume we want to estimate  $\mu = \mathbb{P}(A)$  for some rare event A.
- Crude Monte Carlo: simulates the model directly.
- Estimation

$$\mu \approx \hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n X_i$$

where the  $X_i$  are i.i.d. copies of Bernoulli r.v.  $X = 1_A$ . •  $\sigma[X_i] = \mu(1 - \mu)$  for a Bernoulli r.v.

# Inefficiency of crude Monte Carlo: relative error

• Confidence interval

$$\left(\hat{\mu}_n-c_{\alpha}\sqrt{\frac{\mu(1-\mu)}{n}},\ \hat{\mu}_n+c_{\alpha}\sqrt{\frac{\mu(1-\mu)}{n}}\right)$$

estimated by

$$\left(\hat{\mu}_n-c_{\alpha}\sqrt{rac{\hat{\mu}_n(1-\hat{\mu}_n)}{n}},\ \hat{\mu}_n+c_{\alpha}\sqrt{rac{\hat{\mu}_n(1-\hat{\mu}_n)}{n}}
ight)$$

• Relative half width  $c_{\alpha}\sigma/(\sqrt{n}\mu) = c_{\alpha}\sqrt{(1-\mu)/\mu/n} \to \infty$  as  $\mu \to 0$ .

• For a given relative error RE, the min required value of

$$n=c_{\alpha}^{2}\frac{1-\mu}{RE^{2}\mu},$$

thus inversely proportional to  $\mu$ .

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Inefficiency of crude Monte Carlo: occurence of the event

- To get a single occurence, we need in average  $1/\mu$  replications (10<sup>9</sup> for  $\mu = 10^{-9}$ ).
- If no observation the returned interval is (0,0)
- Otherwise, if (unlikely) one observation when  $n \ll 1/\mu$ , over-estimation of mean and variance
- In general, bad coverage of the confidence interval unless  $n \gg 1/\mu$ .
- As we can see, something has to be done to accelerate the occurence (and reduce variance).
- An estimator has to be "robust" to the rarity of the event.

Modelling analysis of robustness: parameterisation of rarity

- In rare-event simulation models, we often parameterize with a rarity parameter  $\epsilon > 0$  such that  $\mu = \mathbb{E}[X(\epsilon)] \rightarrow 0$  as  $\epsilon \rightarrow 0$ .
- Typical example
  - For a direct Bernoulli r.v.  $X = 1_A$ ,  $\epsilon = \mu = \mathbb{E}[1_A]$ .
  - When simulating a system involving failures and repairs, e can be the rate or probability of individual failures.
  - ▶ For a queue or a network of queues, when estimating the overflow probability,  $\epsilon = 1/C$  inverse of the capacity of the considered queue.
- The question is then: how behaves an estimator as  $\epsilon \rightarrow 0$ , i.e., the event becomes rarer?

Robustness properties: Bounded relative error (BRE)

- An estimator X(ε) is said to have bounded relative variance (or bounded relative error) if σ<sup>2</sup>(X(ε))/μ<sup>2</sup>(ε) is bounded uniformly in ε. Equivalent to saying that σ(X(ε))/μ(ε) is bounded uniformly in ε.
- Interpretation: estimating  $\mu(\epsilon)$  with a given relative accuracy can be achieved with a bounded number of replications even if  $\epsilon \to 0$ .
- When the confidence interval comes from the central limit theorem, it means that the relative half width

$$c_{\alpha} \frac{\sigma(X(\epsilon))}{\sqrt{n}}$$

remains bounded as  $\epsilon \rightarrow 0$ .

# Robustness properties: Asymptotic Optimality (AO)

- BRE has often been found difficult to verify in practice (ex: queueing systems).
- Weaker property: asymptotic optimality (or logarithmic efficiency) if

$$\lim_{\epsilon \to 0} \frac{\ln(\mathbb{E}[X^2(\epsilon)])}{\ln(\mu(\epsilon))} = 2.$$

- Equivalent to say that  $\lim_{\epsilon \to 0} \ln(\sigma^2[X(\epsilon)]) / \ln(\mu(\epsilon)) = 2$ .
- Property also called *logarithmic efficiency* or *weak efficiency*.
- Quantity under limit is always positive and less than or equal to 2:  $\sigma^2[X(\epsilon)] \ge 0$ , so  $\mathbb{E}[X^2(\epsilon)] \ge (\mu(\epsilon))^2$  and then  $\ln \mathbb{E}[X^2(\epsilon)] \ge 2 \ln \mu(\epsilon)$ , i.e.,

$$\frac{\ln \mathbb{E}[X^2(\epsilon)]}{\ln \mu(\epsilon)} \leq 2.$$

• Interpretation: the second moment and the square of the mean go to zero at the same *exponential* rate.

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## Relation between BRE and AO

- AO weaker property: if we have BRE,  $\exists \kappa > 0$  such that  $\mathbb{E}[X^2(\epsilon)] \leq \kappa^2 \mu^2(\epsilon)$ , i.e.,  $\ln \mathbb{E}[X^2(\epsilon)] \leq \ln \kappa^2 + 2 \ln \mu(\epsilon)$ , leading to  $\lim_{\epsilon \to 0} \ln \mathbb{E}[X^2(\epsilon)] / \ln \mu(\epsilon) \geq 2$ . Since this ratio is always less than 2, we get the limit 2.
- Not an equivalence. Some counter-examples:
  - an estimator for which γ = e<sup>-η/ε</sup> with η > 0, but for which the variance is Q(1/ε)e<sup>-2η/ε</sup> with Q a polynomial;
  - exponential tilting in queueing networks.
- Other robustness measures exist (based on higher degree moments, on the Normal approximation, on simulation time...)

### Work-normalized properties

- Variance is not all, generation time is important (figure of merit).
- Let σ<sub>n</sub><sup>2</sup>(ε) and t<sub>n</sub>(ε) be the variance and generation time t<sub>n</sub>(ε) for a sample of size n.
- When t<sub>n</sub>(ε) is strongly dependent on ε, any behavior is possible: increasing or decreasing to 0 as ε → 0.
- Work-normalized versions of the above properties:
  - The estimator verifies work-normalized relative variance if

$$\frac{\sigma_n^2(\epsilon)t_n(\epsilon)}{\mu^2(\epsilon)}$$

is upper-bounded whatever the rarity, and is therefore a work-normalized version of the bounded relative error property.

The estimator verifies work-normalized asymptotic optimality if

$$\lim_{\epsilon \to 0} \frac{\ln t_n(\epsilon) + \ln \sigma_n^2(\epsilon)}{\ln \mu(\epsilon)} = 2.$$

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# Outline

#### Introduction

- 2 Monte Carlo: the basics
- Inefficiency of crude Monte Carlo, and robustness issue

#### Importance Sampling

#### 5 Splitting

6 Confidence interval issues

# Importance Sampling (IS)

- Let X = h(Y) for some function h where Y obeys some probability law ℙ.
- $\bullet$  IS replaces  $\mathbb P$  by another probability measure  $\tilde{\mathbb P},$  using

$$E[X] = \int h(y)d\mathbb{P}(y) = \int h(y)\frac{d\mathbb{P}(y)}{d\tilde{\mathbb{P}}(y)}d\tilde{\mathbb{P}}(y) = \tilde{\mathbb{E}}\left[h(Y)L(Y)\right]$$

- $L = d\mathbb{P}/d\mathbb{P}$  likelihood ratio,
- $\blacktriangleright~\tilde{\mathbb{E}}$  is the expectation associated with probability law  $\tilde{\mathbb{P}}.$
- Required condition:  $d\tilde{\mathbb{P}}(y) \neq 0$  when  $h(y)d\mathbb{P}(y) \neq 0$ .
- If  $\mathbb{P}$  and  $\tilde{\mathbb{P}}$  continuous laws, L ratio of density functions  $f(y)/\tilde{f}(y)$ .

$$E[X] = \int h(y)f(y)dy = \int h(y)\frac{f(y)}{\tilde{f}(y)}\tilde{f}(y)dy = \tilde{\mathbb{E}}\left[h(Y)L(Y)\right].$$

• If  $\mathbb{P}$  and  $\tilde{\mathbb{P}}$  are discrete laws, L ratio of indiv. prob  $p(y_i)/\tilde{p}(y_i)$ 

$$E[X] = \sum_{i} h(y_i) p(y_i) = \sum_{i} h(y_i) \frac{p(y_i)}{\tilde{p}(y_i)} \tilde{p}(y_i) = \tilde{\mathbb{E}} \left[ h(Y) L(Y) \right].$$
### Estimator and goal of IS

Take (Y<sub>i</sub>, 1 ≤ i ≤ n) i.i.d; copies of Y, according to P. The estimator is

$$\frac{1}{n}\sum_{i=1}^{n}h(Y_i)L(Y_i).$$

• The estimator is unbiased:

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}h(Y_i)L(Y_i)\right] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left[h(Y_i)L(Y_i)\right] = \mu.$$

 $\bullet$  Goal: select probability law  $\tilde{\mathbb{P}}$  such that

$$\tilde{\sigma}^2[h(Y)L(Y)] = \tilde{\mathbb{E}}[(h(Y)L(Y))^2] - \mu^2 < \sigma^2[h(Y)].$$

• It means changing the probability distribution such tat the 2nd moment is smaller.

#### IS difficulty: system with exponential failure time

- Y: exponential r.v. with rate  $\lambda$ .
- A = "failure before T" = [0, T].
- Goal: compute  $\mu = \mathbb{E}[1_A(Y)] = 1 e^{-\lambda T}$ .
- $\bullet$  Use for IS an exponential density with a different rate  $\tilde{\lambda}$

$$\widetilde{\mathbb{E}}[(1_{\mathcal{A}}(Y)\mathcal{L}(Y))^{2}] = \int_{0}^{T} \left(\frac{\lambda e^{-\lambda y}}{\tilde{\lambda} e^{-\tilde{\lambda} y}}\right)^{2} \widetilde{\lambda} e^{-\tilde{\lambda} y} dy = \frac{\lambda^{2}(1 - e^{-(2\lambda - \tilde{\lambda})T})}{\widetilde{\lambda}(2\lambda - \tilde{\lambda})}.$$

• Variance ratio for T = 1 and  $\lambda = 0.1$ :



• If  $A = [T, \infty)$ , i.e.,  $\mu = \mathbb{P}[Y \ge T]$ , and IS with exponential with rate  $\tilde{\lambda}$ :  $\tilde{\mathbb{E}}[(\mathbf{1}_{A}(Y)\mathcal{L}(Y))^{2}] = \int_{T}^{\infty} \left(\frac{\lambda e^{-\lambda y}}{\tilde{\lambda}e^{-\tilde{\lambda}y}}\right)^{2} \tilde{\lambda}e^{-\tilde{\lambda}y}dy = \frac{\lambda^{2}e^{-(2\lambda-\tilde{\lambda})T}}{\tilde{\lambda}(2\lambda-\tilde{\lambda})}.$ 

• Minimal value computable, but infinite variance wen  $\tilde{\lambda} > 2\lambda$ . If  $\lambda = 1$ :



Optimal estimator for estimating  $\mathbb{E}[h(Y)] = \int h(y)L(y)d\tilde{\mathbb{P}}(y)$ 

• Optimal change of measure:

$$\widetilde{\mathbb{P}} = rac{|h(Y)|}{\mathbb{E}[|h(Y)|]} d\mathbb{P}.$$

 Proof: for any alternative IS measure P', leading to the likelihood ratio L' and expectation E',

 $\tilde{\mathbb{E}}[(h(Y)L(Y))^2] = (\mathbb{E}[|h(Y)|])^2 = (\mathbb{E}'[|h(Y)|L'(Y)])^2 \le \mathbb{E}'[(h(Y)L'(Y))^2].$ 

- If h≥ 0, Ẽ[(h(Y)L(Y))<sup>2</sup>] = (E[h(Y)])<sup>2</sup>, i.e., σ<sup>2</sup>(h(Y)L(Y)) = 0. That is, IS provides a zero-variance estimator.
- Implementing it requires knowing  $\mathbb{E}[|h(Y)|]$ , i.e. what we want to compute; if so, no need to simulation!
- But provides a hint on the general form of a "good" IS measure.

# IS for a discrete-time Markov chain (DTMC) $\{Y_j, j \ge 0\}$

- $X = h(Y_0, ..., Y_{\tau})$  function of the sample path with
  - P = (P(y, z) transition matrix,  $\pi_0(y) = \mathbb{P}[Y_0 = y]$ , initial probabilities
  - up to a stopping time  $\tau$ , first time it hits a set  $\Delta$ .
  - $\mu(y) = \mathbb{E}_{y}[X].$
- IS replaces the probabilities of paths  $(y_0, \ldots, y_n)$ ,

$$\mathbb{P}[(Y_0,\ldots,Y_{\tau})=(y_0,\ldots,y_n)]=\pi_0(y_0)\prod_{j=1}^{n-1}P(y_{j-1},y_j),$$

by  $\widetilde{\mathbb{P}}[(Y_0,\ldots,Y_{\tau})=(y_0,\ldots,y_n)]$  st  $\widetilde{\mathbb{E}}[\tau]<\infty.$ 

For convenience, the IS measure remains a DTMC, replacing P(y, z) by P̃(y, z) and π<sub>0</sub>(y) by π̃<sub>0</sub>(y).

• Then 
$$L(Y_0, \ldots, Y_{\tau}) = \frac{\pi_0(Y_0)}{\tilde{\pi}_0(Y_0)} \prod_{j=1}^{\tau-1} \frac{P(Y_{j-1}, Y_j)}{\tilde{P}(Y_{j-1}, Y_j)}.$$

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#### Illustration: a birth-death process

- Markov chain with state-space  $\{0, 1, \dots, B\}$ ,  $P(y, y + 1) = p_y$  and  $P(y, y 1) = 1 p_y$ , for  $y = 1, \dots, B 1$
- $\Delta = \{0, B\}$ , and let  $\mu(y) = \mathbb{P}[Y_{\tau} = B \mid Y_0 = y]$ .
- Rare event if B large or the pys are small.
- If  $p_y = p < 1$  for y = 1, ..., B 1, known as the gambler's ruin problem.
- An M/M/1 queue with arrival rate λ and service rate μ > λ fits the framework with p = λ/(λ + μ).
- How to apply IS: increase the p<sub>y</sub>s to p̃<sub>y</sub> to accelerate the occurence (but not too much again).
- Large deviation theory applies here, when B increases.
  - $\blacktriangleright$  Strategy for an  ${\rm M}/{\rm M}/{\rm 1}$  queue: exchange  $\lambda$  and  $\mu$
  - Asymptotic optimality, but no bounded relative error.

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#### Zero-variance IS estimator for Markov chains simulation

• Restrict to an additive (positive) cost

$$X = \sum_{j=1}^{\tau} c(Y_{j-1}, Y_j)$$

Is there a Markov chain change of measure yielding zero-variance?Yes we have zero variance with

$$\tilde{P}(y,z) = \frac{P(y,z)(c(y,z) + \mu(z))}{\sum_{w} P(y,w)(c(y,w) + \mu(w))} \\
= \frac{P(y,z)(c(y,z) + \mu(z))}{\mu(y)}.$$

• Without the additivity assumption the probabilities for the next state must depend in general of the entire history of the chain.

#### Zero-variance for Markov chains

• Proof by induction on the value taken by  $\tau$ , using the fact that  $\mu(Y_{\tau}) = 0$  In that case, if  $\tilde{X}$  denotes the IS estimator,

$$\begin{split} \tilde{X} &= \sum_{i=1}^{\tau} c(Y_{i-1}, Y_i) \prod_{j=1}^{i} \frac{P(Y_{j-1}, Y_j)}{\tilde{P}(Y_{j-1}, Y_j)} \\ &= \sum_{i=1}^{\tau} c(Y_{i-1}, Y_i) \prod_{j=1}^{i} \frac{P(Y_{j-1}, Y_j) \mu(Y_{j-1})}{P(Y_{j-1}, Y_j) (c(Y_{j-1}, Y_j) + \mu(Y_j))} \\ &= \sum_{i=1}^{\tau} c(Y_{i-1}, Y_i) \prod_{j=1}^{i} \frac{\mu(Y_{j-1})}{c(Y_{j-1}, Y_j) + \mu(Y_j)} \\ &= \mu(Y_0) \end{split}$$

- Unique Markov chain implementation of the zero-variance estimator.
- Again, implementing it requires knowing μ(y) ∀y, the quantities we wish to compute.
- Approximation to be used.

#### Zero-variance approximation

- Use a heuristic approximation μ̂(·) and plug it into the zero-variance change of measure instead of μ(·).
- More efficient but also more requiring technique: *learn adaptively* function  $\mu(\cdot)$ , and still plug the approximation into the zero-variance change of measure formula instead of  $\mu(\cdot)$ .
  - Adaptive Monte Carlo (AMC) proceeds iteratively.
    - ★ Considers several steps and *n<sub>i</sub>* independent simulation replications at step *i*.
    - \* At step *i*, replaces  $\mu(x)$  by a guess  $\mu^{(i)}(x)$
    - use probabilities

$$\tilde{P}_{y,z}^{(i)} = \frac{P_{y,z}(c_{y,z} + \mu^{(i)}(z))}{\sum_{w} P_{y,w}(c_{y,w} + \mu^{(i)}(w))}.$$

\* Gives a new estimation  $\mu^{(i+1)}(y)$  of  $\mu(y)$ , from which a new transition matrix  $\tilde{P}^{(i+1)}$  is defined.

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# Adaptive stochastic approximation (ASA)

- ASA just uses a single sample path  $(y_0, \ldots, y_n)$ .
- Initial distribution for  $y_0$ , matrix  $\tilde{P}^{(0)}$  and guess  $\mu^{(0)}(\cdot)$ .
- At step j of the path, if  $y_j \not\in \Delta$ ,
  - matrix  $\tilde{P}^{(j)}$  used to generate  $y_{j+1}$ .
  - From  $y_{j+1}$ , update the estimate of  $\mu(y_j)$  by

$$\begin{aligned} \mu^{(j+1)}(y_j) &= (1-a_j(y_j))\mu^{(j)}(y_j) \\ &+ a_j(y_j) \left[ c(y_j,y_{j+1}) + \mu^{(j)}(y_{j+1}) \right] \frac{P(y_j,y_{j+1})}{\tilde{P}^{(j)}(y_j,y_{j+1})}. \end{aligned}$$

where  $\{a_j(y), j \ge 0\}$ , sequence of *step sizes* 

- For  $\delta > 0$  constant,  $\tilde{P}^{(j+1)}(y_j, y_{j+1}) = \max\left(P(y_j, y_{j+1}) \frac{[c(y_j, y_{j+1}) + \mu^{(j+1)}(y_{j+1})]}{\mu^{(j+1)}(y_j)}, \delta\right).$ Otherwise  $\mu^{(j+1)}(y) = \mu^{(j)}(y), \tilde{P}^{(j+1)}(y, z) = P^{(j)}(y, z).$ Normalize:  $P^{(j+1)}(y_j, y) = \frac{\tilde{P}^{(j+1)}(y_j, y)}{\sum_{i=1}^{n} \tilde{P}^{(j+1)}(y_i, z)}.$
- If  $y_j \in \Delta$ ,  $y_{j+1}$  generated from initial distribution, but estimations of  $P(\cdot, \cdot)$  and  $\mu(\cdot)$  kept.
- Batching techniques used to get a confidence\_interval.

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### Drawbacks of the learning techniques

- You have to store vectors  $\mu^{(n)}(\cdot)$ . State-space typically very large when we use simulation...
- This limits the practical effectiveness of the method.
- Other possibility:
  - Use K basis functions  $\mu^{(1)}(\cdot), \ldots, \mu^{(K)}(\cdot)$ , and an approximation

$$\mu(\cdot) \equiv \sum_{k=1}^{K} \alpha_k \mu^{(k)}(\cdot).$$

- Learn coefficients α<sub>k</sub> as in previous methods, instead of the function itself.
- See also how best basis functions can be learnt, as done in dynamic programming.

### Illustration of heuristics: birth-death process

- Let P(i, i + 1) = p and P(i, i 1) = 1 p for  $1 \le i \le B 1$ , and P(0, 1) = P(B, B 1) = 1.
- We want to compute μ(1), probability of reaching B before coming back to 0.
- If p small, to approach  $\mu(\cdot)$ , we can use

$$\hat{\mu}(y) = p^{B-y} \quad \forall y \in \{1, \dots, B-1\}$$

with  $\hat{\mu}(0) = 0$  and  $\hat{\mu}(B) = 1$  based on the asymptotic estimate  $\mu(i) = p^{B-i} + o(p^{B-i})$ .

• We can verify that the variance of this estimator is going to 0 (for fixed sample size) as  $p \rightarrow 0$ .

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# Other procedure: optimization within a parametric class

- No direct relation with the zero-variance change of measure.
- Parametric class of IS measures depending on vector θ, {ℙ<sub>θ</sub>, θ ∈ Θ}:
   family of densities f<sub>θ</sub>, or of discrete probability vectors p<sub>θ</sub>.

Find

 $\theta^* = \operatorname{argmax}_{\theta} \mathbb{E}_{\theta}[(h(Y)L(Y))^2].$ 

- The optimization can sometimes be performed analytically
  - Ex: estimate  $\mu = \mathbb{P}[X \ge na]$  for X Binomial(n, p)
  - IS parametric family  $Binomial(n, \theta)$ .
  - Twisting the parameter p to  $\theta = a$  is optimal (from Large Deviations theory).

# Adaptive learning of the best parameters

- The value of  $\theta$  that minimize the variance can be learned adaptively in various ways.
- ASA method can be adapted to optimize  $\theta$  by stochastic approximation.
- We may replace the variance in the optimization problem by some distance between P
  <sub>θ</sub> and the optimal dP
  <sup>\*</sup> = (|X|/E[|X|])dP, simpler to optimize.
- Cross-entropy technique uses the Kullback-Leibler "distance"

$$egin{aligned} \mathcal{D}( ilde{\mathbb{P}}^*,\, ilde{\mathbb{P}}_ heta) &= & ilde{\mathbb{E}}^*\left[\lograc{d ilde{\mathbb{P}}^*}{d ilde{\mathbb{P}}_ heta}
ight] \ &= & \mathbb{E}\left[rac{|X|}{\mathbb{E}[|X|]}\log\left(rac{|X|}{\mathbb{E}[|X|]}d\mathbb{P}
ight)
ight] - rac{1}{\mathbb{E}[|X|]}\mathbb{E}\left[|X|\log d ilde{\mathbb{P}}_ heta
ight]. \end{aligned}$$

Determine then

$$\max_{\theta\in\Theta}\mathbb{E}\left[|X|\log d\tilde{\mathbb{P}}_{\theta}\right] = \max_{\theta\in\Theta}\tilde{\mathbb{E}}\left[\frac{d\mathbb{P}}{d\tilde{\mathbb{P}}}|X|\log d\tilde{\mathbb{P}}_{\theta}\right].$$

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# Adaptive learning in Cross-Entropy (CE)

- CE method applied in an iterative manner, increasing the rarity at each step.
- Start with  $\theta_0 \in \Theta$  and r.v.  $X_0$  whose expectation is easier to estimate than X.
- At step  $i \ge 0$ ,  $n_i$  independent simulations are performed using IS with  $\theta_i$ , to approximate the previous maximization ( $\tilde{\mathbb{P}}$  replaced by  $\tilde{\mathbb{P}}_{\theta_i}$ )
- Solution of the corresponding sample average problem

$$heta_{i+1} = \arg \max_{ heta \in \Theta} rac{1}{n_i} \sum_{j=1}^{n_i} |X_i(\omega_{i,j})| \log(d\tilde{\mathbb{P}}_{ heta}(\omega_{i,j})) rac{d\mathbb{P}}{d\tilde{\mathbb{P}}_{ heta_i}}(\omega_{i,j}),$$

where  $\omega_{i,j}$  represents the *j*th sample at step *i*.

• Kullback-Leibler distance is convenient for the case where  $\tilde{\mathbb{P}}_{\theta}$  is from an exponential family, because the log and the exponential cancel.

# Outline

#### Introduction

- 2 Monte Carlo: the basics
- Inefficiency of crude Monte Carlo, and robustness issue
- Importance Sampling

#### 5 Splitting

6 Confidence interval issues

# Splitting: general principle

- Splitting is the other main rare event simulation technique.
- Assume we want to compute the probability  $\mathbb{P}(D)$  of an event D.
- General idea:
  - Decompose

$$D_1 \supset \cdots \supset D_m = D,$$

- Use P(D) = P(D<sub>1</sub>)P(D<sub>2</sub> | D<sub>1</sub>) · · · P(D<sub>m</sub> | D<sub>m-1</sub>), each conditional event being "not rare",
- Estimate each individual conditional probability by crude Monte Carlo, i.e., without changing the laws driving the model.
- The final estimate is the product of individual estimates.
- Question: how to do it for a stochastic process? Difficult to sample conditionally to an intermediate event.

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# Graphical interpretation



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Splitting and Markov chain  $\{Y_j; j \ge 0\} \in \mathcal{Y}$ 

• Goal: compute  $\gamma_0 = \mathbb{P}[\tau_B < \tau_A]$  with

• 
$$\tau_A = \inf\{j > 0 : Y_{j-1} \notin A \text{ and } Y_j \in A\}$$

• 
$$\tau_B = \inf\{j > 0 : Y_j \in B\}$$

• Intermediate levels from importance function  $h: \mathcal{Y} \to \mathbb{R}$  with  $A = \{x \in \mathcal{Y} : h(x) \le 0\}$  and  $B = \{x \in \mathcal{Y} : h(x) \ge \ell\}$ :

Partition [0, ℓ) in m subintervals with boundaries
 0 = ℓ<sub>0</sub> < ℓ<sub>1</sub> < · · · < ℓ<sub>m</sub> = ℓ.

• Let 
$$T_k = \inf\{j > 0 : h(Y_j) \ge \ell_k\}$$
 and  $D_k = \{T_k < \tau_A\}$ .

#### Ist stage:

- simulate  $N_0$  chains until min $(\tau_A, T_1)$ .
- ▶ If  $R_1$  number of chains for which  $D_1$  occurs,  $\hat{p}_1 = R_1/N_0$  unbiased estimator of  $p_1 = \mathbb{P}(D_1)$ .
- Stage 1 < k ≤ m:</p>
  - If  $R_{k-1} = 0$ ,  $\hat{p}_l = 0$  for all  $l \ge k$  and the algorithm stops
  - Otherwise, start N<sub>k</sub> chains from these R<sub>k</sub> entrance states, by potentially cloning (splitting) some chains
  - simulate these chains up to  $\min(\tau_A, T_k)$ .
  - $\hat{p}_k = R_k / N_{k-1}$  unbiased estimator of  $p_k = \mathbb{P}(D_k | D_{k-1})$

### Two-dimensional illustration



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# The different implementations

- Fixed splitting:
  - clone each of the R<sub>k</sub> chains reaching level k in c<sub>k</sub> copies, for a fixed positive integer c<sub>k</sub>.
  - $N_k = c_k R_k$  is random.
- Fixed effort:
  - ► *N<sub>k</sub>* fixed a priori
  - ► random assignment draws the N<sub>k</sub> starting states at random, with replacement, from the R<sub>k</sub> available states.
  - *fixed assignment*, on the other hand, we would split each of the R<sub>k</sub> states approximately the same number of times.
  - ▶ Fixed assignment gives a smaller variance than random assignment because it amounts to using stratified sampling over the empirical distribution *G<sub>k</sub>* at level *k*.
- Fixed splitting can be implemented in a depth-first way, recursively, while fixed effort cannot.
- On the other hand, you have no randomness (less variance) in the number of chains with fixed effort.

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# Diminishing the computational effort

- As k increases, it is likely that the average time before reaching the next level or going back to A increases significantly.
- We can kill (truncate) trajectories hat go a given number β of levels down (unlikely to come back), but biased.
- Unbiased solution: apply the Russian roulette principle
  - ▶ kill the trajectory going down with a probability  $r_{\beta}$ . If it survives, assign a multiplicative weight  $1/(1 r_{\beta})$ .
  - Several possible implementations to reduce the variance due to the introduction of weights.

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#### Issues to be solved

- How to define the importance function h?
  - If the state space is one-dimensional and included in ℝ, the final time is an almost surely finite stopping time and the critical region is B = [b,∞), any strictly increasing function would be good (otherwise a mapping can be constructed, by just moving the levels), such as for instance h(x) = x.
  - If the state space is multidimensional: the importance function is a one-dimensional projection of the state space.
  - Desirable property: the probability to reach the next level should be the same, whatever the entrance state in the current level.
  - Ideally, h(x) = P[τ<sub>B</sub> ≤ τ<sub>A</sub> | X(0) = x], but as in IS, they are a probabilities we are looking for.
  - ► This h(·) can also be learnt or estimated a priori, with a presimulation, by partitionning the state space and assuming it constant on each region.

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# Issues to be solved (2)

- How many offsprings at each level?
  - In fixed splitting:
    - \* if  $c_k < 1/p_k$ , we do not split enough, it will become unlikely to reach the next event;
    - \* if  $c_k > 1/p_k$ , the number of trajectories will exponentially explode with the number of levels.
    - \* The right amount is  $c_k = 1/p_k$  ( $c_k$  can be randomized to reach that value if not an integer).
  - In fixed effort, no explosion is possible.
  - In both cases, the right amount has to be found.
- How many levels to define?
  - i.e., what probability to reach the next level?

### **Optimal values**

- In a general setting, very few results exist:
  - ▶ We only have a central limit theorem based on genetic type interacting particle systems, as the sample increases.
  - Nothing exist on the definition of optimal number of levels...
- Consider the simplified setting, with a single entrance state at each level.
- Similar to coin-flipping to see if next level is reached or not.
- In that case, asymptotically optimal results can be derived, providing hints of values to be used.

Simplified setting and fixed effort

• 
$$N_0 = N_1 = \dots = N_{m-1} = n$$

- The  $\hat{p}_k$ 's binomial r.v. with parameters n and  $p_k = p = \mu_0^{1/m}$  assumed independent.
- It can be shown that

$$\begin{aligned} \operatorname{Var}[\hat{p}_{1}\cdots\hat{p}_{m}] &= \prod_{k=1}^{m} \mathbb{E}[\hat{p}_{k}^{2}] - \gamma_{0}^{2} = \left(p^{2} + \frac{p(1-p)}{n}\right)^{m} - p^{2m} \\ &= \frac{mp^{2m-1}(1-p)}{n} + \cdots + \frac{(p(1-p))^{m}}{n^{m}}. \end{aligned}$$

• Assuming 
$$n \gg (m-1)(1-p)/p$$
,  
 $\operatorname{Var}[\hat{p}_1 \cdots \hat{p}_m] \approx mp^{2m-1}(1-p)/n \approx m\gamma_0^{2-1/m}/n$ .

- The work normalized variance  $\approx [\gamma_0^n m^2]/n = \gamma_0^{2-1/m} m^2$
- Minimized at  $m = -\ln(\gamma_0)/2$
- This gives  $p^m = \gamma_0 = e^{-2m}$ , so  $p = e^{-2}$ .
- But the relative error and its work-normalized version both increase toward infinity at a logarithmic rate.
- There is no asymptotic optimality either.

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# Simplified setting: fixed splitting

- $N_0 = n$ ,  $p_k = p = \gamma_0^{1/m}$  for all k, and c = 1/p; i.e.,  $N_k = R_k/p$ .
- The process  $\{N_k, k \ge 1\}$  is a branching process.
- From standard branching process theory

$$\operatorname{Var}[\hat{p}_1\cdots\hat{p}_m]=m(1-p)p^{2m-1}/n.$$

- If p fixed and  $m \to \infty$ , the squared relative error m(1-p)/(np) is unbounded,
- But it is asymptotically efficient:

$$\lim_{\gamma_0 \to 0^+} \frac{\log(\mathbb{E}[\tilde{\gamma}_n^2])}{\log \gamma_0} = \lim_{\gamma_0 \to 0^+} \frac{\log(m(1-p)\gamma_0^2/(np) + \gamma_0^2)}{\log \gamma_0} = 2.$$

• Fixed splitting is asymptotically better, but it is more sensitive to the values used.

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Illustrative simple example: a tandem queue

- Illustrative of the impact of the importance function.
- Two queues in tandem
  - arrival rate at the first queue is  $\lambda = 1$
  - mean service time is  $\rho_1 = 1/4$ ,  $\rho_2 = 1/2$ .
  - ► Embedded DTMC: Y = (Y<sub>j</sub>, j ≥ 0) with Y<sub>j</sub> = (Y<sub>1,j</sub>, Y<sub>2,j</sub>) number of customers in each queue after the *j*th event
  - $B = \{(x_1, x_2) : x_2 \ge L = 30\}, A = \{(0, 0)\}.$
- Goal: impact of the choice of the importance function?
- Importance functions:

$$\begin{array}{lll} h_1(x_1, x_2) &=& x_2, \\ h_2(x_1, x_2) &=& (x_2 + \min(0, x_2 + x_1 - L))/2, \\ h_3(x_1, x_2) &=& x_2 + \min(x_1, L - x_2 - 1) \times (1 - x_2/L). \end{array}$$

### Illustration, fixed effort: a tandem queue (2)

- $V_N$ : variance per chain, (N times the variance of the estimator) and the work-normalized variance per chain,  $W_N = S_N V_N$ , where  $S_N$  is the expected total number of simulated steps of the N Markov chains.
- With  $h_1$ ,  $\hat{V}_N$  and  $\hat{W}_N$  were significantly higher than for  $h_2$  and  $h_3$ .
- Estimators rescaled as  $\tilde{V}_N = 10^{18} \times \hat{V}_N$  and  $\tilde{W}_N = 10^{15} \times \hat{W}_N$ .

	$N = 2^{10}$		$N = 2^{12}$		$N = 2^{14}$		$N = 2^{16}$	
	$\tilde{V}_N$	$\tilde{W}_N$	$\tilde{V}_N$	$\tilde{W}_N$	$\tilde{V}_N$	ŴΝ	$\tilde{V}_N$	$\tilde{W}_N$
h <sub>2</sub> , Splitting	109	120	89	98	124	137	113	125
h <sub>2</sub> , Rus. Roul.	178	67	99	37	119	45	123	47
h <sub>3</sub> , Splitting	93	103	110	121	93	102	107	118
$h_3$ , Rus. Roul.	90	34	93	35	94	36	109	41

# Outline

#### Introduction

- 2 Monte Carlo: the basics
- Inefficiency of crude Monte Carlo, and robustness issue
- Importance Sampling

#### 5 Splitting

6 Confidence interval issues

# Confidence interval issues

- Robustness is an issue, but what about the confidence interval validity?
- If the rare event has not occured: empirical confidence interval is (0,0).
- The problem can even be more underhand: it may happen that the rare event happens due to some trajectories, but other important trajectories important for the variance estimation are still rare and not sampled: the empirical confidence confidence interval is not good then.

# Illustrative example of the difficulty



- 4-component system with two classes of components, subject to failures and repairs. Discrete time Markov Chain

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# IS probability used

• Failure Biasing scheme: for each up state  $\neq$  (2, 2), we increase the probability of failure to the constant q (ex: 0.8) and use individual probabilities proportional to the original ones.



#### Empirical evaluation as $\epsilon \rightarrow 0$

• Fix the number of samples,  $n = 10^4$ , using the same pseudo-random number generator, and varying  $\varepsilon$  from  $10^{-2}$  down to 0.

• Remember that 
$$\mu = 2\epsilon^2 + o(\epsilon^2)$$
 and  $\sigma_{IS}^2 = \Theta(\epsilon^3)$ .

$\epsilon$	$2\epsilon^2$	Est.	Confidence Interval	Est. RE
1e-02	2e-04	2.03e-04	(1.811e-04,2.249e-04)	1.08e-01
1e-03	2e-06	2.37e-06	(1.561e-06, 3.186e-06)	3.42e-01
2e-04	8e-08	6.48e-08	(1.579e-08, 1.138e-07)	7.56e-01
1e-04	2e-08	9.95e-09	(9.801e-09, 1.010e-08)	1.48e-02
1e-06	2e-12	9.95e-13	(9.798e-13, 1.009e-12)	1.48e-02
1e-08	2e-16	9.95e-17	(9.798e-17, 1.009e-16)	1.48e-02

• The estimated value becomes bad as  $\epsilon \rightarrow 0$ .

It seems that BRE is verified while it is not!

#### Asymptotic explanation

- When  $\varepsilon$  small, transitions in  $\Theta(\varepsilon)$  not sampled anymore.
- Asymptotic view of the Markov chain:



# Asymptotic explanation (2)

- For this system:
  - the expectation is  $\epsilon^2 + o(\epsilon^2)$
  - variance  $\frac{1-q^2}{nq^2}\varepsilon^4 + o(\epsilon^4)$ .
- Results in accordance to the numerical values, and BRE is obtained.
- But does not correspond to the initial system, with different values.
- Reason: important paths are still rare under this IS scheme.
- Diagnostic procedures can be imagined.
### PART II: APPLICATIONS

Tutorial on Monte Carlo techniques, DEPEND 2010, Venezia, 19/7/10

## OUTLINE

- 1. HRMS (Highly Reliable Markovian Systems): IS examples
- 2. STATIC MODELS (Network Reliability):
  - a) a recursive variance reduction technique
  - b) reducing time instead of variance

#### 1/ HRMS: IS examples



# MODEL

- Very used in dependability analysis of complex systems
- Simplified version and description here
- System is composed of components belonging to C classes
- Components are either up or down
- The whole system is also either up or down
- Failures and repairs (of any component) are exponentially distributed
- CTMC  $Y = (Y_1, ..., Y_c)$  where  $Y_c$  is the number of up components in class c



- There is a (structure) function saying for any value of Y if the system's state is up or down
- Let  $\Delta$  be the set of down states
- Let 1 be the state where all components are up, the initial state of Y
- Goal: evaluate  $\mu$  = Pr(hitting  $\Delta$  before 1)
- This is an important metric in dependability analysis (and also in performance issues)



- Usual situation: at some time scale, failure rates are in  $O(\epsilon)$  and repairs in O(1)
- To estimate  $\mu$ , we can
  - move to the canonically embedded DTMC
  - and use the standard Monte Carlo approach
- In the DTMC, failure probabilities are in O(ε) (except for state 1) and repair ones in O(1)
- Idea: use Importance Sampling



# Failure Biaising (FB)

- Also sometimes called Simple Failure Biaising
- Probably the simplest idea
- Idea: just push the system towards  $\Delta$  by changing the (small) failure probabilities into something "not small"
- For any state  $x \neq 1$  in the DTMC,
  - we change the total (the sum) of the corresponding failure probabilities to some constant q (typically 0.5 < q < 0.8)</li>
  - and we distribute it proportionally to the original values

## FB example

#### first order (in $\epsilon$ ) expressions



FB

#### symbolically, for an operational state $x \neq 1$



This technique works but it does not have the BRE property



#### **Balanced FB**



This version does have the BRE property



# Selective FB (SFB)

- Let us call initial a failure event consisting in the first failure in some class of components.
- Accordingly, a secondary failure is any other failure event.
- Intuitively, it seems a good idea to give more "weight" to secondary failures, expecting to reach set ∆ quicker this way.
- This leads to the Selective Biasing scheme shown in next slide.



#### SFB

#### symbolically, for an operational state $x \neq 1$



This technique works but it does not have the BRE property

### **Balanced SFB**



This technique does have the BRE property

## SFBS: SFB for Series-like sys

- Always the same idea: take advantage of available information, if possible.
- Here, we assume that not only we know if failures are initial or not, but also, we know that the system's structure is "series-like".
- The typical example is a series of k-out-of-n modules. Denote the parameters of module i as k<sub>i</sub>, n<sub>i</sub>.
- We define as critical the failure of a component in a module *i* such that after it, we have  $Y_i k_i = \min_j (Y_j k_j)$ .

SFBS

#### symbolically, for an operational state $x \neq 1$



This technique works but it does not have the BRE property

### **Balanced SFBS**



This technique does have the BRE property

## Other ideas

- Other ideas have been published and shown to be effective (names are not "standardized"):
  - SFBP: SFB for Parallel-like systems
    - similar to SFBS but for systems composed of a set of modules working in parallel
  - DSFB: Distance-based SFB
    - for systems where it is possible to evaluate with almost no cost the distance from any up state to  $\Delta$
  - IDSFB: Inverse-Distance-based SFB
    - an improvement of DSFB
  - IFB: Inverse SFB
    - a method based on the optimal IS c.o.m. for the M/M/1 queuing model
  - and others ...





- The zero variance idea in IS leads to very efficient methods for this HRMS family of models.
- Recall that in this approach, we consider the probability  $\mu_x$  of hitting  $\Delta$  before **1**, starting from any state x of the chain.
- Some existing results:
  - methods with BRE
  - even "vanishing relative error" obtained, when the approximation of  $\mu_x$  can use all paths from x to  $\Delta$  with smallest degree in  $\epsilon$ .





- Numerical results so far are impressive with these techniques (in terms of efficiency and also of stability).
- For instance, in a model with 20 classes of components, with 4 components per class, and the working criterion "system is up iff at least 7 components are up", a typical result is

METHOD	BFB	0 var
μ	3.1 .10-11	3.0 10-11
Var	8.5 10 <sup>-18</sup>	1.3 10-24
CPU time	11 sec	97 sec

#### 2a/ A RECURSIVE VARIANCE REDUCTION TECHNIQUE FOR STATIC PROBLEMS



## ABSTRACT

- A variance-reduction procedure for network reliability estimation
- Main ideas:
  - exploit the specificities of the problem (graph theory concepts, binary coherent structures)
  - improve efficiency by including exact computations into the Monte Carlo procedure
- More specifically:
  - a recursive decomposition-based approach
  - using two basic concepts in the considered family of systems: paths and cuts



## OUTLINE

- introduction
- some graph concepts
- the method
- some results



## 1 NETWORK RELIABILITY







## REFERENCE MODEL

A COMMUNICATION NETWORK





### REFERENCE MODEL

A COMMUNICATION NETWORK





## REFERENCE MODEL

#### A COMMUNICATION NETWORK



- nodes are perfect
- lines behave independently
- lines are up or down
- for each line i,
   r<sub>i</sub> = Pr(line i is up)

Associated key-words:

- reliability diagrams, fault-trees...
- graph theory, coherent binary structure theory

# MODEL

- V: the nodes K: the terminals, or target-set,  $K \subseteq V$ E: the lines or edges  $\{r_i\}_{i \text{ in } E}$ : the elementary reliabilities
- N = (V, E): (the underlying) undirected graph (also called the *network* when we include the probabilities associated with the edges)



## RANDOM STRUCTURE

- Set of all partial sub-graphs of N (same nodes, part of the edges)
- G = (V, F): a random graph on  $\Omega$ ; probabilistic structure: for any  $H \subseteq E$ ,  $Pr(G = (V, H)) = \prod_{i \in H} r_i \prod_{j \notin H} (1 - r_j)$



## METRIC

- goal: R = K-network reliability, = Pr(the nodes in K are connected) (or equivalently Q = 1 - R)
- U: set of all partial sub-graphs of N where all nodes in K are connected; thus, R = Pr(G in U)
- usual situation:  $R \sim 1$ , that is,  $Q \sim 0$
- only MC can handle medium/large models; but possible problem: the rare event situation



## 2 STANDARD MC

The rare event problem when  $Q \ll 1$ 



## COMPUTATIONAL COMPLEXITY

- Internal loop: sampling a graph state (state of each edge), and verifying if it belongs or not to set U (DFS search); total complexity is O(|E|).
- *M* iterations; initialization time and final computations in O(1).
- Total computation time in O(M|E|), linear in # of edges and # of replications.

## ACCURACY

- the correct answer given by the MC method is not "unreliability is Q" but "unreliability belongs with high probability to (Q1, Q2)"
- more precisely, here is a possible output "routine":
  - Pr(  $Q \in (Q1, Q2)$ )  $\approx 0.95$
  - $Q1 = Q^{\text{std}} 1.96 V^{\text{std}}$ ,  $Q2 = Q^{\text{std}} + 1.96 V^{\text{std}}$
  - V<sup>std</sup> = StandardEstimator(Variance(Q<sup>std</sup>))

=  $[Q^{\text{std}}(1 - Q^{\text{std}})/(M - 1)]^{1/2}$ 

- relative error in the answer: RelErr = 1.96 V<sup>std</sup>/Q<sup>std</sup> = [(1 - Q<sup>std</sup>)/((M-1) Q<sup>std</sup>]<sup>1/2</sup> ≈ 1/(MQ<sup>std</sup>)<sup>1/2</sup> which is problematic when Q<sup>std</sup> « 1
- Variance Reduction Techniques: estimation methods such that the variance of the estimators (and their own estimators) are smaller than the variance of the crude estimator.



#### "SOME TRIVIAL CASES"







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### 3 SERIES-PARALLEL REDUCTIONS






















 $r_2 r_3 + r_4 - r_2 r_3 r_4$ 

Series-parallel reductions have polynomial cost.



### 4 PATHS AND CUTS



#### A PATH (|K| = 2)





### A CUT (|K| = 2)





#### A PATH (|K| = 4)





### A CUT (|K| = 4)



- Let *P* be a path.
- Let P-up denote the event
   P-up = "all links in P are up",
   Pr(P-up) = ∏<sub>link i is in P</sub> r<sub>i</sub>
- Since P-up  $\Rightarrow$  system is up, Pr(P-up)  $\leq R$
- Let C be a cut.
- Let C-down denote the event C-down = "all links in C are down", Pr(C-down) =  $\prod_{link \ i \ is \ in \ C} (1 - r_i)$
- Since C-down  $\Rightarrow$  system is down, Pr(C-down)  $\leq Q = 1 - R$

# 5 THE GENERAL IDEA

 Again, with P be a path and P-up the event "all links in P are up", we can write R = Pr(P-up) + [1 - Pr(P-up)] Pr(sys. up | "at

least one link in P is down")

 This suggest to sample on a conditional system, to estimate the last conditional probability (idea used in previous works by the authors).



- Here, we follow another conditioning-based idea coming also from previous works (the RVR estimator).
- We define an estimator Z associated with our MC method which is illustrated here through examples:
  - if the network is



- then















• The remaining case is a K-connected network where there is no possible series-parallel reduction and  $|K| \ge 2$ .





We first select a path\*:



Let  $L_i$  be the event "line *i* is up", and let  $\underline{L}_i$  be the event "line *i* is down", *i* = 1,2.

\* The RVR method used a cut, but the idea is the same.



• We partition  $\boldsymbol{\varOmega}$  in the following way:

$$\Omega = \{L_1 L_2, \underline{L_1}, L_1 \underline{L_2}\}$$
Prob. =  $r_1 r_2$ 
Prob. =  $1 - r_1$ 

• Let X be the r.v. "first line down in the path", i = 1,2, with X = 0 if all lines in the path are up.

- Let Y = X | X > 0 (Y lives in {1,2})
- We have  $Pr(Y = 1) = (1 r_1) / (1 r_1 r_2)$ and  $Pr(Y = 2) = r_1(1 - r_2) / (1 - r_1 r_2)$ .









to evaluate Zhere,







# 6 THE METHOD (SKETCH)

- It consists of generalizing this idea to work with a path and a cut simultaneously.
- Assume we select a cut  $C = (l_1, l_2, l_3)$  and a path  $P = (l_1, l'_2, l'_3)$ (paper's notation here).
- Denote by L<sub>i</sub> (resp. by L'<sub>i</sub>) the event "link I<sub>i</sub> is up" (resp. "link I'<sub>i</sub> is up"), and by L<sub>i</sub> (resp. by L'<sub>i</sub>) the event "link I<sub>i</sub> is down" (resp. "link I'<sub>i</sub> is down").
- Consider we partition first  $\Omega$  into the events  $\{L_1L'_2L'_3, L_1, L_1L'_2, L_1L'_2L'_3\}$ , that is, the events
  - "all 3 links in P work",
  - "link  $l_1$  of P is down"
  - "in P, link  $l_1$  is up and link  $l_2$  is down"
  - "in P, links  $I_1$  and  $I_2$  are up and link  $I_3$  is down"









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• Now, we refine the partition crossing the previous decomposition with the partition  $\{L_1L_2L_3, L_1, L_1L_2, L_1L_2L_3\}$ , using now cut *C*.

















- Remark: the only sampled variables are the  $Y_k$  (the auxiliary variable at the *k*th irreducible and not trivial network found in the recursive process)
- THEOREM
  - E(Z) = Q (so, unbiaised estimator)
  - Var(Z) ≤ [R Pr(P-up)][Q Pr(C-down)] ≤ RQ (so, variance reduction)



## 7 EXAMPLE: the bridge



 $M = 10^6$  samples

•  $r_1 = 1 - \exp(-1/0.3) \sim 0.964326$ •  $r_2 = 1 - \exp(-1/0.1) \sim 0.999955$ •  $r_3 = 1 - \exp(-1/0.8) \sim 0.713495$ •  $r_4 = 1 - \exp(-1/0.1) \sim 0.999955$ •  $r_5 = 1 - \exp(-1/0.2) \sim 0.993262$ ( $R \sim 0.999929$ )

Var(Q<sup>std</sup>)/Var'(Q<sup>re</sup>) ~ 1.95×10<sup>6</sup> (Var'(Q<sup>×</sup>) is the variance Var'(Q<sup>ce</sup>)/Var'(Q<sup>re</sup>) ~ 187 of the considered estimator x of Q) a recent cross-entropy-based estimator

# 7 EXAMPLE: the 3-grid



 $M = 10^6$  samples

$q_i = 1 - r_i$	Q	Var(Q <sup>std</sup> )/ Var'(Q <sup>re</sup> )	Var'(Q <sup>ce</sup> )/ Var'(Q <sup>re</sup> )
10-3	~ 4.00×10 <sup>-12</sup>	~ 4.49×10 <sup>5</sup>	~ 2.07
10-6	~ 4.00×10 <sup>-18</sup>	~ 4.44×10 <sup>11</sup>	~ 2.06



## 7 EXAMPLE: the 6-grid

|V|



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<b>q</b> <sub>i</sub>	Q	Var(Q <sup>std</sup> )/ Var'(Q <sup>re</sup> )	Var'(Q <sup>ce</sup> )/ Var'(Q <sup>re</sup> )
10-3	~ 4.01×10 <sup>-6</sup>	~ 1.13×10 <sup>5</sup>	~ 1.06
10-6	~ 4.00×10 <sup>-12</sup>	~ 1.11×10 <sup>11</sup>	~ 1.04

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## 7 EXAMPLE: the 10-complete graph

- We varied K(|K| = 2, |K| = 5, |K| = 10) and we considered always the case  $r_i = r$  varying r from 0.99 to 0.1.
- Main goal of the experiments: evaluate the improvement of working with both a cut and a path, compared to the original technique that used only a cut.
- For instance, the ratio between the variance of the estimator using only a cut and the variance of the new one goes from ~ 2 when |K| = 10 and r = 0.1 to ~ 10<sup>27</sup> when |K| = 2 and r = 0.99.



## 7 EXAMPLE: the dodecahedron



Here, we took always the case of |K| = 2 but varied the distance between the two terminals (in the picture, that distance is 5).


- We also varied  $r_i = r$  from 0.99 to 0.1.
- When the distance is 1, the ratio between the variance of the estimator using only a cut and the variance of the new one goes from ~  $3.8 \times 10^3$  if r = 0.99 to ~  $9.2 \times 10^7$  if r = 0.1.
- At the other extreme, when the distance was 5, the method using only a cut was slightly better in the case of r = 0.99; for the remaining values of r the ratio ranged in the interval  $\sim (2.4, 4.6)$ .



## 8 CONCLUSIONS

- The method is simple and efficient (so far it compares well with previous proposals, while this must be explored more in deep).
- It can be extended to more powerful decompositions.
- More importantly, the choice of the cut and the path is not evident (because of the transformations made to the graphs when simplifying them inside the recursive procedure).



#### 2b/ IMPROVING EFFICIENCY BY TIME REDUCTION (INSTEAD OF VARIANCE REDUCTION)



### ABSTRACT

- A time-reduction procedure for network reliability estimation
- Main idea:
  - again, exploit the specificities of this static problem
  - a version of conditional Monte Carlo
- For simplicity, and because we are probably close to out of time at this point, we consider only the source-to-terminal case



## 2 STANDARD MC

The rare event problem when  $Q \ll 1$ 



#### COMPUTATIONAL COMPLEXITY

- Internal loop: sampling a graph state (state of each edge), and verifying if it belongs or not to set U (DFS search); total complexity is O(|E|).
- *M* iterations; initialization time and final computations in O(1).
- Total computation time in O(M|E|), linear in # of edges and # of replications.

# MAIN IDEA

- Imagine we implement the crude Monte Carlo procedure in the following way:
  - first, we build a (huge) table with M rows (e.g.  $M = 10^9$ ) and |E| + 1 columns
  - each row corresponds to a replication
  - row *m*:
    - column *i*: 1 if edge *i* works at repl. *m*, 0 otherwise
    - last column (|E| + 1): 1 if sys. ok, 0 otherwise
  - then, we count the # of 0 in last column, we divide by M and we have our estimator Q<sup>std</sup>



- We consider the case of case  $r_i \approx 1$
- Look at column *i* now: full of '1', from time to time a '0'
- Call F<sub>i</sub> the r.v. "first row in the table with a '0' in column i"
- Assume the table is infinite: in that case,  $F_i$ is geometric on  $\{1, 2, ...\}$  with  $Pr(F_i = f) = r_i^{f-1} (1 - r_i)$ and

$$E(F_i) = r_i / (1 - r_i)$$



- This suggests the following procedure:
  - sample the geometric r.v.  $F_1$ ,  $F_2$ , ... and compute  $W = \min\{F_1, F_2, ...\}$
  - consider that in replications 1, 2, ..., W-1, the system was operational
  - for replication *W*, perform the DFS test
  - then, start again for each column (edge), sampling the next 'O' value, then looking for the next row with at least one 'O'...
- Formalizing this procedure we can prove that it can be seen as an implementation of the standard estimator



# COMPLEXITY ISSUE

- For a table with *M* rows,
  - each  $F_i$  is sampled, on the average,  $M/E(F_i)$  times, thus, the total cost is

$$M\sum_{i}\frac{1-r_i}{r_i}$$

- in the rare event case, the usual situation is  $(1 - r_i)/r_i \ll 1$  and even

$$\sum_{i} \frac{1 - r_i}{r_i} \ll 1$$



• # of calls to the DFS procedure?

- on the average, M/E(W) times

- Since W is also geometric with parameter  $r = r_1 r_2 \dots r_{|E|}$ , the mean cost of the method is  $M\left(\sum_i \frac{1-r_i}{r_i} + |E| \frac{1-r}{r}\right)$
- For instance, assume  $r_i = 1 \varepsilon$
- The total mean cost is ~  $\varepsilon M |E|^2$



• Dividing the mean cost of the standard approach M |E| by the mean cost of this more efficient "implementation", we get  $1/(\varepsilon |E|)$ 

#### ILLUSTRATIONS

• Consider the following example:



source = 1 terminal = 14  $r_i = 0.9999$ 

the new method runs ~ 500 times faster than crude (for the same accuracy)

# FINAL COMMENTS

- The procedure can be improved further
- For instance, the DFS can be called only if the number of '0' in the row is at least equal to the breadth of the graph
- In the previous example, this leads to an improvement factor of ~ 600

TUTORIAL'S CONCLUSIONS



- Many other techniques, applications and problems, not even mentioned here.
- Some randomly chosen examples:
  - use of Quasi-Monte Carlo techniques
  - using other types of information
  - splitting with static models
  - applications in physics (where "everything was invented...")
- Slides will be on-line with some added bibliography



 Reference:
G. Rubino, B. Tuffin (Editors), "Rare Event Simulation Using Monte Carlo Methods" John Wiley & Sons, 278 pages, March 2009.
<a href="http://eu.wiley.com/WileyCDA/WileyTitle/productCd-0470772697.html">http://eu.wiley.com/WileyCDA/WileyTitle/productCd-0470772697.html</a>

