#### Importance Splitting for Rare Event Estimation

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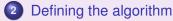
UNC Chapel Hill, February 22, 2010

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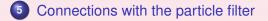








#### 4 Examples



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The Problem Setup

## The problem

Computing the probability of rare events for Markov models arises in many applications, e.g.

- Buffer overflow in queueing models
- Transitions between different modes of the stationary distribution in stochastic kinetic models.

Typical probabilities are in the range  $10^{-6} - 10^{-20}$ . Naive Monte Carlo produces estimates equal to zero even with long simulations. Want the relative mean square error to be bounded.

Importance sampling can be used, but constructing good proposal distributions where weights have small variance is difficult.

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The Problem Setup

## Importance splitting

Importance splitting (Garvels and Kroese 1998, Glasserman et al. 1999, Garvels 2000, L'Ecuyer et al. 2006) is an attractive alternative, based on "divide and conquer".

Write the event of interest E as the last member in a decreasing sequence of m events

$$D_m = E \subset D_{m-1} \subset \ldots \subset D_0 = \Omega$$

Then

$$P(E) = \prod_{k=1}^{m} p_k$$
 where  $p_k := P(D_k \mid D_{k-1}) = \frac{P(D_k)}{P(D_{k-1})}$ 

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and we estimate  $p_k$  for each k.

The Problem Setup

## Rare events in Markov models

- $(X_t)$  Markov process on *E* (discrete or continuous time).
- Starting point *x*<sup>0</sup> fixed (unless stated otherwise).
- *A*, *B* two disjoint subsets of *E*,  $x_0 \notin B$ , often  $x_0 \in A$ .
- $\tau$  = first hitting time of *B*,  $\xi$  = first time *X*<sub>t</sub> (re)enters *A*.
- Want to know  $\gamma := P(\tau < \xi)$

Other choices of  $\xi$  are possible, e.g. a fixed time  $t_0$ , but make notation more complicated.

# Defining the sets $D_k$

- Choose an importance function  $\Phi : E \to \mathbb{R}$  with  $A = \{x; \Phi(x) \le 0\}, B = \{x; \Phi(x) \ge 1\}.$
- Choose *m* and levels  $I_0 = \Phi(x_0) < I_1 < ... < I_m = 1$ .
- Let  $\tau_k$  = first hitting time of  $\{x; \Phi(x) \ge l_k\}$  and  $D_k = \{\tau_k < \xi\}$ .
- For later use, define also  $\mu_k = \text{law of } X_{\tau_k}$  given  $D_k$

In particular,  $\tau_0 = 0$ ,  $\mu_0$  is the point mass in  $x_0$  and  $\tau_m = \tau$ .

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## The recursive algorithm

- Assume we have a sample of size  $N_k$  from  $\mu_k$ .
- Simulate independent chains starting at each point of this sample until min(τ<sub>k+1</sub>, ξ) and let R<sub>k+1</sub> be the number of chains where τ<sub>k+1</sub> < ξ.</li>
- If  $R_{k+1} = 0$ , set  $\widehat{\gamma} = 0$  and stop.
- Otherwise

$$\widehat{p_{k+1}} = \frac{R_{k+1}}{N_k}$$

and inflate the sample of the  $R_{k+1}$  values of  $X_{\tau_{k+1}}$  to a sample of size  $N_{k+1}$ . (Ties will disappear in the next step of the recursion)

## Sample inflation strategies

- Fixed splitting:  $N_{k+1} = c_{k+1}R_{k+1}$  with  $c_{k+1}$  given.
- Fixed effort, random inflation: N<sub>k+1</sub> given, inflation by sampling with replacement
- Fixed effort, balanced inflation:  $N_{k+1}$  given, take each value  $[N_{k+1}/R_{k+1}]$  times plus a sample without replacement
- Fixed number of successes (our proposal): *R<sub>k+1</sub>* ≥ 2 given, sample with replacement at the level *k* until this is achieved. Need to use

$$\widehat{p_{k+1}} = \frac{R_{k+1}-1}{N_k-1}$$

(the UMVU estimator for the negative binomial)

## Choice of the importance function

Bad choices of  $\Phi$  make importance splitting fail! Garvels et al. (2002) propose

$$\Phi(x) = g(P(\tau < \xi | X_0 = x))$$

with *g* monotone. If we cannot compute  $\gamma$ , we cannot compute this  $\Phi$  either.

If *E* is discrete and  $(X_t)$  time homogeneous, we suggest as approximation of the above

 $\Phi(x) =$  probability of the most likely path from *x* to *B* without entering *A*.

This can be computed by Dijkstra's algorithm. Choice of g equivalent to choice of levels (to be discussed later).

Unbiasedness Fixed number of success vs. fixed effort Choice of levels

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## Unbiasedness

Is  $\hat{p}_k$  unbiased for  $p_k$  ? Is  $\hat{\gamma}$  unbiased for  $\gamma$  ?

The answer is no for the first question, and yes for the second (for all versions above).

Some "Proofs" of unbiasedness of  $\widehat{\gamma}$  have appeared which claim conditional unbiasedness of  $\widehat{p_k}$  given the history up to level k - 1.

Correct proofs for some versions are in Del Moral and Garnier (2005) and Dean and Dupuis (2009). We give a more direct proof for all cases.



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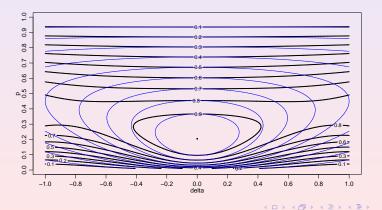
## Advantages of fixed number of successes

- Fixed number of successes controls precision instead of effort.
- Fixed number of successes avoids the problem of returning estimates with the value zero.
- For a single step, fixed number of successes with  $R_k = N_k p_k$  is slightly less efficient than fixed effort.
- For several steps, fixed effort with constant *N<sub>i</sub>* is worse than fixed number of successes with constant *R<sub>i</sub>* if the *p<sub>i</sub>* are different.

Unbiasedness Fixed number of success vs. fixed effort Choice of levels

#### Efficiencies for 2 steps

Efficiency for fixed effort (thin blue line) and fixed number of successes (thick black line) for m = 2,  $p_1 = p^{1+\delta}$ ,  $p_2 = p^{1-\delta}$ .



Unbiasedness Fixed number of success vs. fixed effort Choice of levels

## Analysis assuming conditional independence

Analytic results in general situations are difficult to obtain. We make the simplifying assumption

$$P(D_{k+1}|D_k, X_{\tau_k} = x) = P(D_{k+1}|D_k) = p_k$$
 (a.s.)

Although this is restrictive, it holds if

$$\Phi(x) = P(\tau < \xi | X_0 = x)$$
 and  $\Phi(X_{\tau_k}) = I_k$ 

("the process cannot jump over the levels").

We study how to choose the number of levels *m*, the probabilities  $p_k$  (subject to  $\prod_{k=1}^m p_k = \gamma$ ) and the sample sizes  $N_k$  or  $R_k$ , respectively, to minimze workload *W* for a given relative mean square error *q*.

## Main results

If workload is independent of *m* and *k*, then the optimal solution as  $q \rightarrow 0$  is

$$m = -0.6275..\log(\gamma), \quad p_k \equiv 0.2032...$$

(the exact values can be written with the solution of the equation  $\exp(1/c) = 2c/(2c-1)$ ). Furthermore

$$N_k \equiv n \sim 2.46 rac{-\log(\gamma)}{q}, \quad R_k \equiv r \sim rac{-\log(\gamma)}{2q}$$

Can also express the optimal  $R_k$ 's (or  $N_k$ 's) for given m, q and  $p_1, \ldots, p_m$ .

Unbiasedness Fixed number of success vs. fixed effort Choice of levels

## Implications for the algorithm

Everything unknown at the beginning  $\rightsquigarrow$  Two-stage procedure:

- In the first stage, take many levels and  $R_k \equiv 20$ .
- If the algorithm does not complete in reasonable time, find a better importance function (or buy a faster computer).
- Otherwise, we have initial guesses of *γ* and *p<sub>k</sub>*. If some of the *p<sub>k</sub>* seem close to zero or one, delete or introduce new levels.
- In a second stage, take R<sub>k</sub> ≡ r according to the formulae for optimal choice (where q is now the only tuning constant).
- Alternatively, take  $\sqrt{r}$  replicates of the second stage with  $\sqrt{r}$  number of successes. Average the results and compute a confidence interval by bootstrapping on the log scale.

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The G/G/1 queue The Jackson tandem queue

#### Connections with the particle filter

#### Overflow in the G/G/1 queue

- Weibull inter arrival and service times with shape parameters k<sub>a</sub>, k<sub>s</sub>. Scale parameters λ, μ fixed.
- *X<sub>t</sub>* = (number of customers, remaining time until next arrival, remaining service time).
- $x_0 = (0, 0, 0), A = \{x_1 = 0\}, B = \{x_1 = 104\}.$
- $\Phi(x) = x_1$ .

## Results

100 repetitions of the two-stage procedure above. Nominally  $Var(\hat{\gamma}) = (0.1 \cdot \gamma)^2$ , Workload  $W(\hat{\gamma}) =$  generated random numbers.

k	0.75	1.00	1.25		
$r \approx$	1290	2060	2910		
		$r_k = r$			
$\langle \widehat{\gamma} \rangle$	1.68 · 10 <sup>-6</sup>	$2.22 \cdot 10^{-10}$	$4.40 \cdot 10^{-15}$		
$\widehat{\operatorname{Var}}(\widehat{\gamma})/\langle \widehat{\gamma} \rangle^2$	0.0134	0.0102	0.0116		
$\langle \pmb{W}(\widehat{\gamma})  angle$	7.067 · 10 <sup>6</sup>	$2.254 \cdot 10^{7}$	$5.304 \cdot 10^{7}$		
	$r_k = r^{1/2}$ with averaging				
$\langle \widehat{\gamma} \rangle$	1.66 · 10 <sup>-6</sup>	$2.21 \cdot 10^{-10}$	$4.41 \cdot 10^{-15}$		
$\widehat{\operatorname{Var}}(\widehat{\gamma})/\langle \widehat{\gamma} \rangle^2$	0.0197	0.0124	0.0127		
$\langle W(\widehat{\gamma}) \rangle$	$7.122 \cdot 10^{6}$	2.259 · 10 <sup>7</sup>	5.318 · 10 <sup>7</sup>	2	
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#### Overflow in the Jackson tandem queue

Two queues in series, arrival rate  $\lambda = 1$ , mean service times  $\rho_i = 1/\mu_i$ ,  $\rho_1 = 1/2$ .  $X_t = (X_{1,t}, X_{2,t}) =$  number of customers at both queues,  $x_0 = (0, 0)$ .  $A = \{x_0\}, B = \{x : x_2 \ge 30\}$ . For  $\rho_2 < \rho_1$ , *B* is a rare event. Can compute  $\gamma$  numerically.

Naive importance function  $\Phi(x) = x_2$ , fails. Want  $\Phi(x_1, x_2) < \Phi(x_1 + 1, x_2)$  for small  $x_1$ , because more customers at the first queue make *B* more likely. Our proposal provides this.



## Results

100 repetitions of the two-stage procedure above with the averaged estimator. Nominally  $Var(\hat{\gamma}) = (0.1 \cdot \gamma)^2$ , Workload  $W(\hat{\gamma}) =$  generated random numbers.

ho	1/2	1/3	1/5
$\gamma$	1.86 · 10 <sup>-9</sup>	1.94 · 10 <sup>-14</sup>	8.59 · 10 <sup>-21</sup>
$\langle \widehat{\gamma} \rangle$	1.85 · 10 <sup>-9</sup>	$1.92 \cdot 10^{-14}$	8.58 · 10 <sup>-21</sup>
$\widehat{\operatorname{Var}}(\widehat{\gamma})/\gamma^2$	0.0321	0.0387	0.0340
$\langle W(\widehat{\gamma}) \rangle$	3.704 · 10 <sup>6</sup>	7.495 · 10 <sup>6</sup>	$2.183 \cdot 10^{7}$

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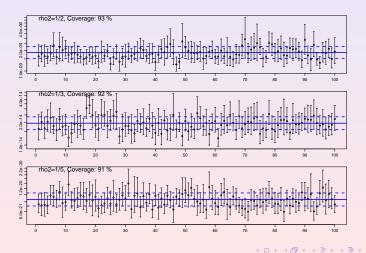
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## 100 Confidence intervals for overflow probability



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Framework Particle filter algorithms Implications

## A general framework (Feynman-Kac)

Want to sample successively from a sequence of target distribution  $\mu_n$  on spaces  $F_n$  which are connected in the following way:

$$\mu_n(dz_n) = \frac{1}{M_n} g_n(z_n) \int_{F_{n-1}} \mu_{n-1}(dz_{n-1}) K_n(z_{n-1}, dz_n)$$

where  $M_n$  is a normalising constant,  $g_n \ge 0$  and  $K_n$  is a transition kernel from  $F_{n-1}$  to  $F_n$ .

Look for weighted samples  $(\zeta_{i,n}, \lambda_{i,n}; i = 1, 2, ..., N)$  that are constructed recursively for computational efficiency.

Framework Particle filter algorithms Implications

## Filtering and smoothing in state space models

 $(Z_t)$  unobserved Markov process, observations  $Y_t$  conditionally independent of  $(Z_s, Y_s; s \neq t)$  given  $Z_t$ .

 $\mu_n$  = conditional distribution of  $Z_n$  given  $Y_1, \ldots, Y_n$  (filtering), is an instance of the general framework if we put  $g_n$  = conditional density of  $Y_n$  given  $Z_n$ ,  $K_n$  = transition kernel of  $Z_n$  given  $Z_{n-1}$ .

For  $\mu_n$  = conditional distribution of  $(Z_0, Z_1, ..., Z_n)$  given  $(Y_1, ..., Y_n)$  (smoothing),  $g_n$  is as above and  $K_n(z_{n-1}, .)$  is a point mass at  $z_{n-1}$  for components 0, 1, ..., n-1 times the transition kernel of  $Z_n$  for the last component.

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#### Importance splitting

Let  $\Delta \notin E$  be an additional (absorbing) state and set

$$Z_n = X_{\tau_n} \mathbf{1}_{[\tau_n < \xi]} + \Delta \mathbf{1}_{[\tau_n > \xi]}.$$

If  $g_n(z) = \mathbf{1}_{[z \neq \Delta]}$ , then  $\mu_n$  is the distribution of  $X_{\tau_n}$  conditioned on  $\tau_n < \xi$ .

In this example, the normalizing constant is  $M_n = P(D_n|D_{n-1})$ , and we want to estimate it. In filtering,  $M_n$  is the conditional density of  $Y_n$  given  $Y_1, Y_2, \ldots, Y_{n-1}$  which is also of interest.

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## The vanilla version of the particle filter

- Resample:  $\zeta_{i,n}^* = \zeta_{j,n}$  with probability  $\lambda_{j,n}$
- Propagate: generate ζ<sub>i,n+1</sub> ~ K<sub>n+1</sub>(ζ<sup>\*</sup><sub>i,n</sub>, dz<sub>n+1</sub>) independently
- Reweight:  $\lambda_{i,n+1} \propto g_{n+1}(\zeta_{i,n+1})$
- Estimate:

$$\widehat{M}_{n+1} = \frac{1}{N} \sum_{i=1}^{N} g_{n+1}(\zeta_{i,n+1})$$

Resampling need not be i.i.d.. It suffices that the expected number of times  $\zeta_{j,n}$  is chosen equals  $N\lambda_{j,n}$ .

Framework Particle filter algorithms Implications

#### More sophisticated versions

For more balanced weights, anticipate the effect of  $g_{n+1}$  at the resampling and propagation steps and adjust the weights:

- Choose a distribution ν for resampling, set J<sub>i</sub> = j with probability ν<sub>j</sub> and ζ<sup>\*</sup><sub>i,n</sub> = ζ<sub>J<sub>i</sub>,n</sub>.
- Choose a kernel *L* for propagation and generate  $\zeta_{i,n+1} \sim L(\zeta_{i,n}^*, dz_{n+1})$  independently,
- Reweight:

$$\lambda_{i,n+1} \propto \frac{\lambda_{J_i,n}}{\nu_{J_i}} \frac{dK_{n+1}(\zeta_{i,n}^*,\zeta_{i,n+1})}{dL(\zeta_{i,n}^*,\zeta_{i,n+1})} g_{n+1}(\zeta_{i,n+1}).$$

Framework Particle filter algorithms Implications

## Implications from the connection

- Use asymptotic results (as number of particles → ∞) for particle filtering to obtain corresponding results for importance splitting.
- In particular, functionals of the path from *x* to *B* given τ < ξ can also be estimated (but need large *N*).
- Particle filtering algorithms show how to combine importance sampling and importance splitting (need to consider the whole path on [τ<sub>n-1</sub>, τ<sub>n</sub>] in order to compute the weights).

- Unbiasedness of estimated normalizing constants is important also for particle filtering (used by Andrieu et al., JRSSB 2010). Notice that it implies that estimated log likelihood is biased.
- Working with random sample sizes to achieve a given effective sample size in the next step could be useful in particle filtering also (less extreme that accept/reject).

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## Thank you for your attention !

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