Fast integration using quasi-random numbers

J. Bossert, M. Feindt, U. Kerzel
University of Karlsruhe
ACAT 05
Outline

- Numerical integration
- Discrepancy
  - The Koksma-Hlawka inequality
- Pseudo- and quasi-random numbers
  - Generators for quasi-random numbers
  - Optimising the discrepancy
  - Quasi-random numbers in $n$ dimensions
  - Comparison
- Examples
Numerical integration

- Integral evaluation using MC technique
  - Integrate integral as expectation value
    \[ \langle f(x) \rangle = \int f(x) \, dx = vol(B) \langle f(x) \rangle \]
  - Estimate \( \langle f(x) \rangle \) by averaging over \( N \) samples:
    \[ \langle f(x) \rangle \approx Q_n f = \frac{1}{N} \sum_i f(x_i) \]
    → use uniformly distributed pseudo-random numbers to sample \( f(x_i) \)
  - Define error: \( \epsilon = |If - Qf| \)
Discrepancy

- measure of roughness
  (deviation from desired flat distribution)
Discrepancy cont...

- in 2 dimensions:

\[ R_N(J) = \left| \frac{A_p(J,N)}{N} - vol(J) \right| \]

- local discrepancy

\[ A_p(J, N) \quad \text{# points in J} \quad N \quad \text{# points in unit square} \]

(number of points in J proportional to ratio of area of J to unit square)

- generalised to s dimensions
Discrepancy cont...

- Discrepancy of a ensemble $P$ with norm:

  - $L_\infty : D^*(P_N) = \sup_{J(x) \in I^s} |R_N(J)|$
  - $L_2 : D^*_2(P_N) = \left( \int_{I^s} (R_N(J))^2 \right)^{\frac{1}{2}}$

\[ D^*_\infty (P_N) \geq D^*_2(P_N) \]

*: one corner of $J$ in (0,0) of unit square

xx May 2005
Ulrich Kerzel, University of Karlsruhe, ACAT 05 - Zeuthen
Koksma-Hlawka inequality

- relates error on numerical integration with discrepancy:

\[ V(f)D_\infty^*(P_N) \geq \epsilon = |If - Qf| \]

- two handles to minimise error \( \epsilon \):
  - minimise variation \( V(f) \) of function \( f \)
    - variable transformation
    - importance sampling
  - sample with numbers with
    - low discrepancy \( D_\infty^*(P_N) \)
Pseudo-random numbers

- follow deterministic pattern
  - created by e.g. linear congruence generator
    \[ y_{i+1} = (ay_i + c) \mod m \rightarrow x_i = y_i/m \]

- statistically independent from each other
  - simulated “real” random numbers
  - Beware of period of generator (e.g. Ranlux: \(10^{165}\))

- Discrepancy:
  \[ D^*_\infty(P_N) = \mathcal{O} \left( \sqrt{\frac{\log \log N}{N}} \right) \rightarrow \mathcal{O} \left( \frac{1}{\sqrt{N}} \right) \]
  \[ \epsilon \propto \frac{1}{\sqrt{N}} \]
Lattice

- 1d: equidistant points have minimal discrepancy

- first idea: extend to s dimensions → lattice

- need $N = n^d$ points
  (otherwise no lattice)

  e.g. $n=4$, $d=2$ → $N=16$
Quasi-random numbers

- constructed to be evenly distributed
- not independent from each other
- need to know total number $N$ from beginning
  - good for integration, not simulation
- low discrepancy series:
  
  $$D^*_\infty = \mathcal{O}\left(\frac{(\log N)^{s-1}}{N}\right)$$

  ⇒ faster convergence, smaller error

$$D^*_\infty(P_N) \rightarrow \mathcal{O}\left(\frac{1}{N}\right)$$

$$\epsilon \propto \frac{1}{N}$$
Quasi-random series

- van der Corput series:
  \[ n = \sum_j d_j b^j ; \quad n = d_N \ldots d_2 d_1 d_0 \]
  
  radially inverse function:
  \[ \varphi_b : \mathbb{N}_0 \to [0, 1) \quad \varphi_b : d_N \ldots d_2 d_1 d_0 \mapsto 0.d_0 d_1 d_2 \ldots d_N \]

  \[ x_n := \varphi_b(n - 1) \]

- other series:
  - **Halton**: extending Corput series to several dimensions
  - **Hammersly**: replace 1\(^{st}\) dim. of Halton series by lattice
    - \( \Rightarrow \) lower discrepancy
(T,M,S) nets and (T,S) series

- **(t,s) series**: class of quasi-random numbers using radically inverse functions with low discrepancy

- **(t,m,s) net**: each elementary interval $E$ ($\text{Vol}(E) = b^{t-m}$) contains $b^t$ points of series with $b^m$ total points

### Example

- **(2,6,2) net:**
  - $2^6 = 64$ total points
  - $2^2 = 4$ points in $E$
Pseudo- vs. Quasi-random

- generate 2048 numbers

![Graphs comparing pseudo-random and quasi-random numbers](image-url)
Comparison

lattice

pseudo-random

quasi-random
Generator examples

Sobol

Faure

Niederreiter

empty structure appears
Optimising discrepancy

- Minima for $N = 2^k$
- “tune” discrepancy by carefully choosing needed $N$
compare discrepancy in several dimensions

→ quasi-random numbers good in few dimensions:

\[ s \approx 2 \ldots 10 \]
Example: Breit-Wigner

numerical integration of multi-dim. BW

\[
\int \prod_{i=1}^{s} \left( \frac{\Gamma_i/2}{\pi((x - x_0)^2 + \Gamma_i^2/4)} \right)
\]

e.g. 2 dimensions:

\[
\begin{array}{cccc}
  x_{01} & x_{02} & \Gamma_1 & \Gamma_2 \\
  44.05 & 57.49 & 10.84 & 8.12 \\
\end{array}
\]

development from real integral value: \((8.8116863 \cdot 10^{-1})\)

<table>
<thead>
<tr>
<th>N</th>
<th>Pseudo</th>
<th>Halton</th>
<th>Faure</th>
<th>Sobol</th>
<th>Niederreiter</th>
<th>Hammersly</th>
<th>Lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>1024</td>
<td>1.03\cdot 10^{-1}</td>
<td>1.72 \cdot 10^{-2}</td>
<td>1.55 \cdot 10^{-2}</td>
<td>1.03 \cdot 10^{-2}</td>
<td>2.36 \cdot 10^{-3}</td>
<td>7.37 \cdot 10^{-4}</td>
<td>4.61 \cdot 10^{-4}</td>
</tr>
<tr>
<td>8192</td>
<td>3.60 \cdot 10^{-2}</td>
<td>1.98 \cdot 10^{-3}</td>
<td>1.94 \cdot 10^{-3}</td>
<td>6.20 \cdot 10^{-4}</td>
<td>1.73 \cdot 10^{-4}</td>
<td>1.24 \cdot 10^{-5}</td>
<td>---------</td>
</tr>
<tr>
<td>16384</td>
<td>2.53 \cdot 10^{-2}</td>
<td>9.08 \cdot 10^{-4}</td>
<td>9.56 \cdot 10^{-4}</td>
<td>2.96 \cdot 10^{-4}</td>
<td>7.11 \cdot 10^{-5}</td>
<td>5.04 \cdot 10^{-6}</td>
<td>9.66 \cdot 10^{-5}</td>
</tr>
</tbody>
</table>
Optimising numerical integration

- **Example**: convolution of BW with resolution per event ($B^0$ mixing analysis)
  - use quasi-random numbers $\Rightarrow$ fewer numbers $N$ needed for evaluation
  - transform for optimal function sampling $\Rightarrow$ importance-sampling
Q-VEGAS

- VEGAS: package for numerical integration in several dimensions:
  - start with uniform intervals
  - evaluate function values in these intervals
  - iteratively adopt interval structure to shape of function

- Q-VEGAS: use quasi-random numbers instead of pseudo-random numbers:
  - faster and more accurate evaluation
Summary

- Low discrepancy (=evenly distributed) numbers important in numerical integration.
- Quasi-random numbers superior in few dimensions:
  - faster convergence
  - higher accuracy

\[ \epsilon \propto \frac{1}{N} \text{ instead of } \frac{1}{\sqrt{N}} \]

- Wide range of applications, e.g. Q-Vegas