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# Multi-armed bandit for stratified sampling: Application to numerical integration

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**Context: numerical integration**

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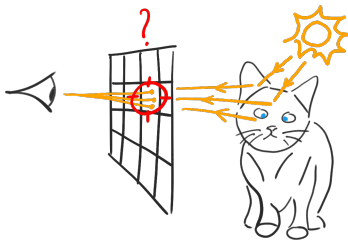
*Artificial intelligence algorithms for image synthesis.*



# It's all about integration

## Image synthesis

We need to compute the *light* received by each pixel.



## Method

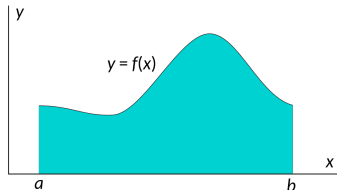
An integration calculation.

$$I = \int_{\mathcal{M} \times S^2} W_e(x, \omega) L_i(x, \omega) dA(x) d\sigma_x^\perp(\omega)$$

$I$  : final colour,  $W_e$  : pixel sensibility,  $L_i$  : incident luminance



**Geometric interpretation** : area under the curve  $y = f(x)$ .



## Notation

$$A = \int_a^b f(x) dx$$

## Applications in high-dimension

- Light transport,
- Brownian motion,
- Analysis of variance (ANOVA) : up to 20D,
- Financial mathematics : up to 360D, ...

[Hah05]

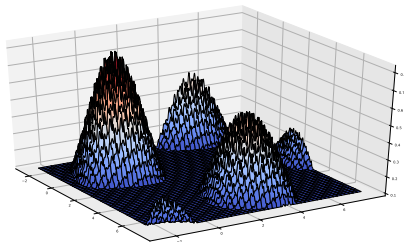
# Solving an integration problem

## Analytical method

$$\text{Antiderivatives: } \int_a^b f(x) dx = F(b) - F(a)$$

### In many cases

The integrand is too difficult. . .



### Numerical methods

- Quadratures
- Sparse grids
- Bayes
- Monte-Carlo

[BOGO15]

# Monte-Carlo methods

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# Vanilla Monte-Carlo

**Idea:** Compute the integral as an *average* of random samples.

## Monte-Carlo

$$\int_0^1 f(x) dx \approx \frac{1}{N} \cdot \sum_{i=1}^N f(x_i)$$

$N$  : number of samples.



- Probabilistic,
- Independent of the dimension,
- Error in  $\mathcal{O}(N^{-1/2})$ ,
- Slow convergence.

[MU49]



# Importance sampling

**Idea:** Focus samples where the integrand seems to be the most interesting.

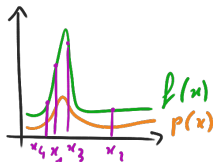
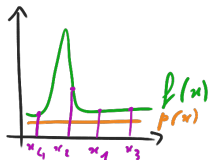
## Importance sampling

$$\int_0^1 f(x) dx \approx \frac{1}{N} \cdot \sum_{i=1}^N \frac{f(x_i)}{p(x_i)}$$

$N$  : number of samples,  $p$  : probability density.

- Faster convergence,
- Improvement when adapting  $p(x)$  through evaluations (Vegas).

[Lep78]



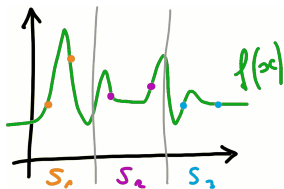
# Stratified sampling

**Idea:** Divide the integrand into strata, then fairly evaluate each stratum.

## Stratified sampling

$$\int_0^1 f(x) dx \approx \sum_{s=1}^S \left( \frac{1}{N_s} \cdot \sum_{i=1}^{N_s} f(x_i) \right)$$

$S$  : number of strata,  $N$  : number of samples per stratum.



- Faster convergence,
- Depends on dimension and on strata cuttings,
- Improvement when adapting strata's *shapes* while evaluating (*Miser*).

[PF90]

# Proposed method based on Machine Learning

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## Machine learning

Methods making a machine evolve from data by a learning-process, in order to solve *difficult* problems.

## Upper Confidence Bound

*Reinforcement* learning, with a trade-off between *exploration* and *exploitation*.



## UCB<sub>1</sub>

$$\text{score}_i = \bar{x}_i + k \times \sqrt{\frac{\ln(N)}{n_i}}$$

$\bar{x}_i$  : arm<sub>i</sub>'s average reward,

$k$  : exploration parameter,

$N$  : total number of pulls,

$n_i$  : arm<sub>i</sub>'s number of pulls.

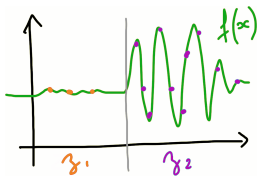
[ACBF02]

# Application to numerical integration

**Idea:** Divide integrand in *zones*, then exploit most interesting zones.

## Expected behaviour

- Evaluate where the integrand varies the most,
- Faster convergence.



## Algorithm

```
initialize zones with stratified sampling  
(low number of samples)
```

```
while we have samples left do  
    determine the best zone (UCB)  
    sample in this zone  
    update variance  
    update number of samples  
    compute new scores
```

```
end
```

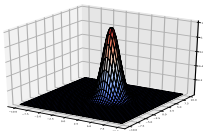
```
compute integral estimation
```

**Multidimensional integrands:** Based on Genz test suite.

[Gen87]

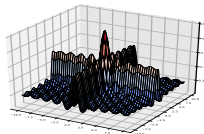
**Gaussian**

$$\exp(-\alpha^2(\mathbf{x} - \beta)^2)$$



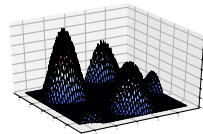
**Cardinal sine**

$$0.2 + \frac{0.8}{N_d} \sum_{i=1}^{N_d} \frac{\sin(\pi \alpha_i x_i)}{\pi \alpha_i x_i}$$



**Noisy card. sin.**

$$\max [0, \sin 2 \cos(\mathbf{T}(\alpha, \beta, \mathbf{x}))]$$



## Parameters

Set for each dimension.

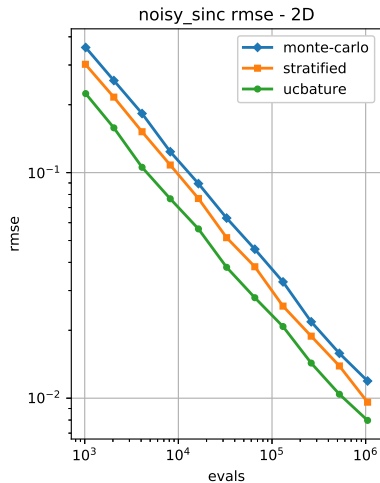
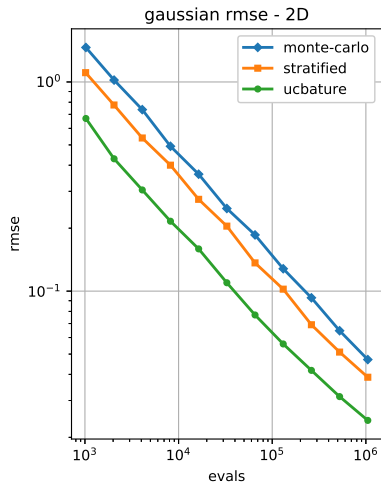
$\alpha$  : integrand difficulty,

$\beta$  : localization in space.

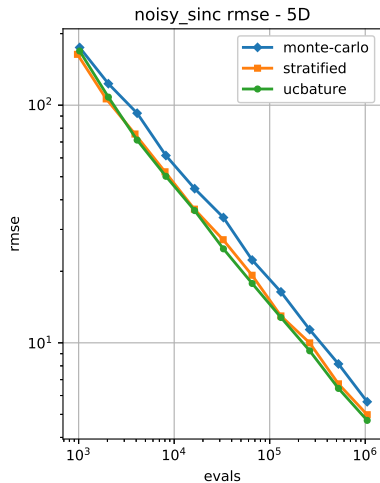
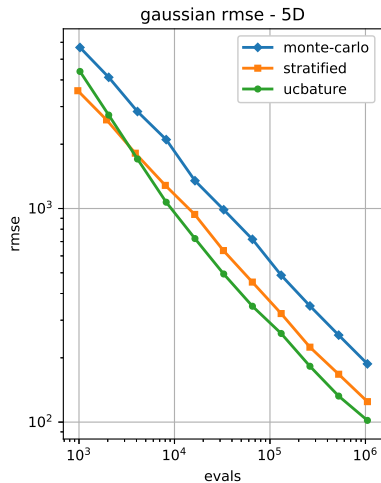
## Experiences

- Randomize integrand,
- Estimate ground truth,
- Compute average error.

# Results (2D integrands)



# Results (5D integrands)





# About parameters

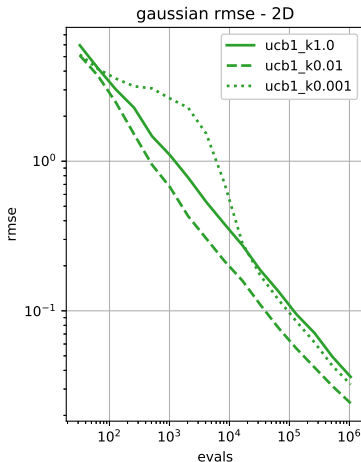
## Difficulty

The exploration parameter  $k$  is hard to determine.

It depends on the integrand, the integration domain, the dimension, the number of divisions. . .

*When good results are obtained in integrating a high-dimensional function, we should conclude first of all that an especially tractable integrand was tried and not that a generally successful method has been found.*

Art Owen — Stanford University



## Proposed method

- Multidimensional numerical integration
- Stratified Monte-Carlo with UCB selection
- Source code: <https://github.com/florianLepretre/ucbature>

## Advantages

- Fast convergence,
- Gains on stratified sampling.

## Limitations

- Parameters tuning,
- High dimensions.

## Future works

- Adapt number of strata and bounds dynamically (*post-stratification*),
- Implement our UCB technique in a *tree* structure (UCT),
- Apply our algorithm on image synthesis problems.

謝謝

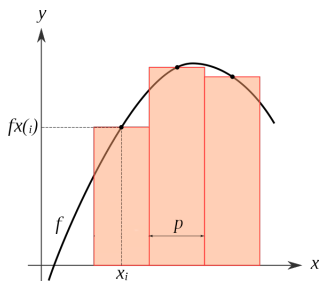
**Thank you.**

**Any questions ?**

## Quadrature

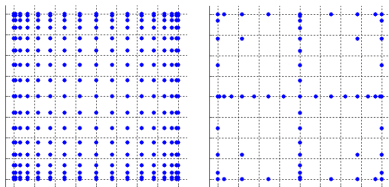
Estimation by constant or polynomial functions.

→ Grows with dimension.  
 $D = 9, N = 10 \rightarrow 10^9$  rectangles



## Sparse grid

Estimation by a tensor product.

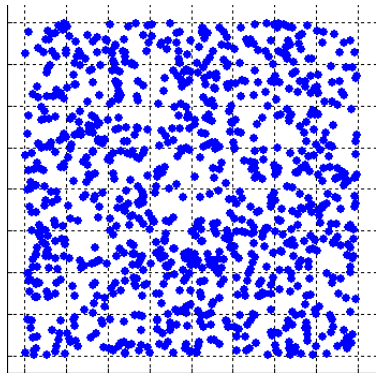


*Equivalent product rule and sparse grid.*

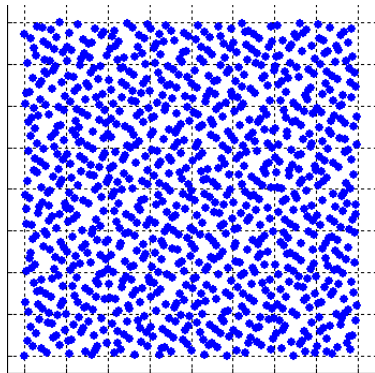
## Bayes

Estimation by inference from likelihood.

# Sampling



Classical **Monte-Carlo** sampling.



**Quasi-Monte-Carlo** sampling.

# Detailed algorithm

## Initialization, main loop, and integral estimation

{initialization using stratified sampling}

```
for  $i \leftarrow 1, N$  do
  for  $k \leftarrow 1, K_{0,i}$  do
    sample  $\mathbf{x}$  in  $C_i$ 
     $\mathbf{y} \leftarrow f(\mathbf{x})$ 
     $S_i \leftarrow S_i + \mathbf{y}$ 
     $S'_i \leftarrow S'_i + \mathbf{y}^2$ 
  end for
end for
```

```
 $k_i \leftarrow K_{0,i}, \forall i$ 
 $V_i \leftarrow \frac{S'_i}{k_i} - \left(\frac{S_i}{k_i}\right)^2, \forall i$ 
```

{multi-armed bandit}

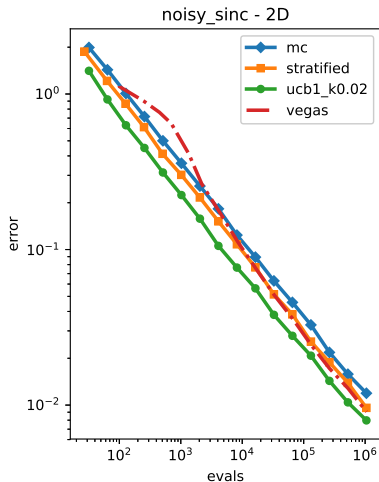
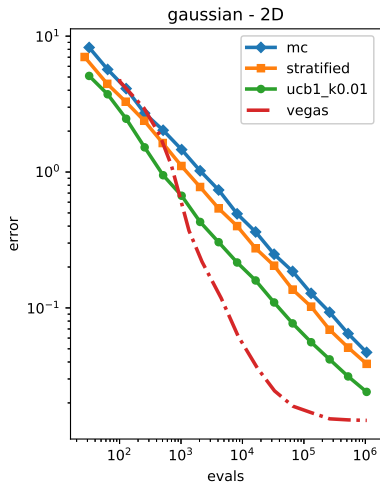
```
for  $k \leftarrow \sum_i^N K_{0,i}, K$  do
   $i \leftarrow \arg \max_i [\text{Ucb}(k, k_i, V_i)]$ 
  sample  $\mathbf{x}$  in  $C_i$ 
   $\mathbf{y} \leftarrow f(\mathbf{x})$ 
   $S_i \leftarrow S_i + \mathbf{y}$ 
   $S'_i \leftarrow S'_i + \mathbf{y}^2$ 
   $k_i \leftarrow k_i + 1$ 
   $V_i \leftarrow \frac{S'_i}{k_i} - \left(\frac{S_i}{k_i}\right)^2, \forall i$ 
end for
```

{final result}

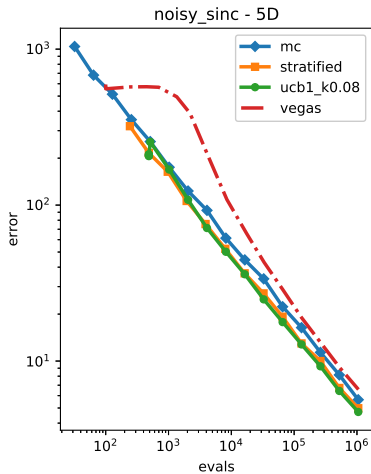
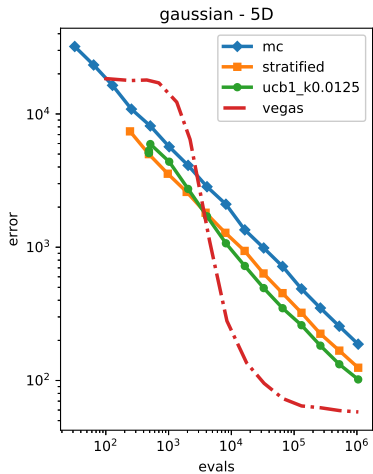
```
 $F' \leftarrow \sum_i^N V_i \frac{S_i}{k_i}$ 
```

**N**: number of *clusters*, **K**<sub>0</sub>: initial evaluations, **K**: maximal evaluations,  
**C**: *clusters*, **V**: *average rewards*, **S**, **S'**: *rewards sums*.

# Comparison to Vegas (2D integrands)



# Comparison to Vegas (5D integrands)







Peter Auer, Nicolò Cesa-Bianchi, and Paul Fischer.

**Finite-time analysis of the multiarmed bandit problem.**

*Mach. Learn.*, 47(2-3):235–256, May 2002.



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**Frank-Wolfe Bayesian Quadrature: Probabilistic Integration with Theoretical Guarantees.**

*ArXiv e-prints*, June 2015.



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**A Package for Testing Multiple Integration Subroutines, pages 337–340.**

Springer Netherlands, Dordrecht, 1987.



T. Hahn.

**Cuba - a library for multidimensional numerical integration.**

*Computer Physics Communications*, 168(2):78 – 95, 2005.



G Peter Lepage.

**A new algorithm for adaptive multidimensional integration.**

*Journal of Computational Physics*, 27(2):192 – 203, 1978.



Nicholas Metropolis and S. Ulam.

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*Journal of the American Statistical Association*, 44(247):335–341,  
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William H. Press and Glennys R. Farrar.

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*Comput. Phys.*, 4(2):190–195, February 1990.

Contextual multi-armed bandits model decision problems, where the properties of the possible decisions are initially partially known, but may become better known as time passes. Such models have numerous applications and many algorithms have been proposed to provide approximate solutions.

In this paper, we propose an algorithm for computing multidimensional integration problems. Such problems are very common and can be solved using the Monte-Carlo method with the stratified sampling technique. This method consists in partitioning the integration domain then randomly sampling the partitions. Our algorithm considers the selection of the best partition to sample as a multi-armed bandit problem, which can be solved using the Upper Confidence Bound technique. We have experimented this approach for several integration problems and observed faster convergence rates.