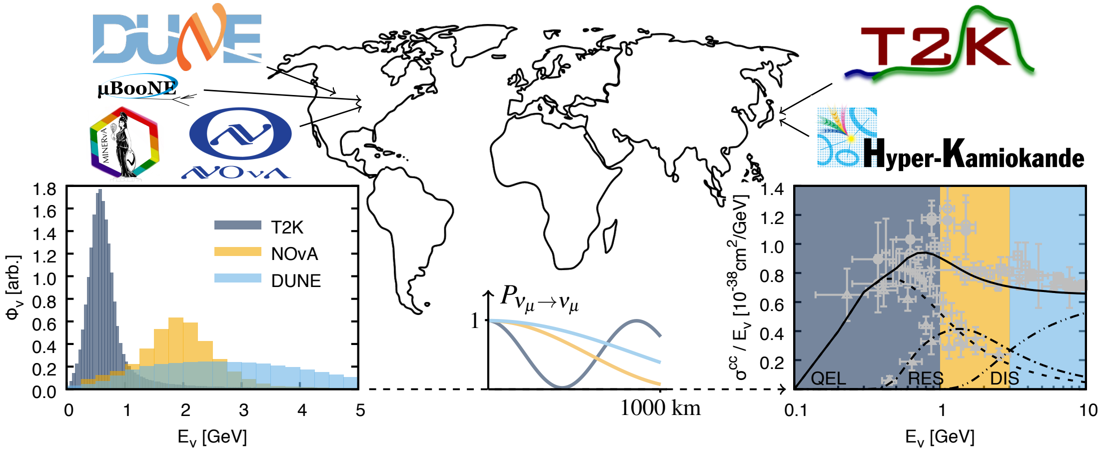
How generators work ...and why it's wrong*

Kajetan Niewczas



$$P(\nu_\mu \to \nu_e) \simeq \sin^2(2\theta)\,\sin^2\left(1.27\frac{\Delta m^2 L}{E_\nu}\right)$$

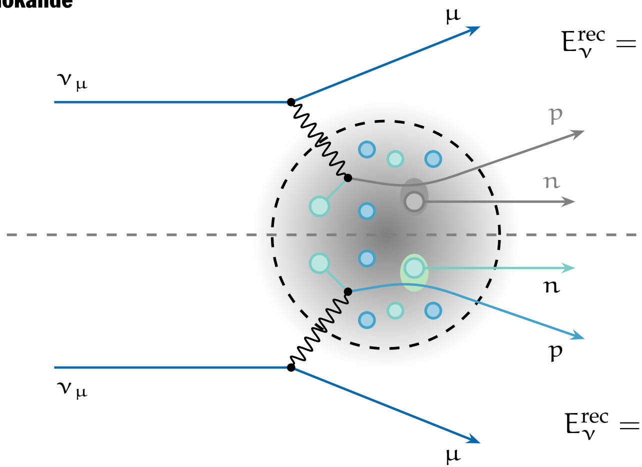
oscillation — amplitude — frequency

$$A_{CP} = \frac{P(\nu_\mu \to \nu_e) - P(\bar{\nu}_\mu \to \bar{\nu}_e)}{P(\nu_\mu \to \nu_e) + P(\bar{\nu}_\mu \to \bar{\nu}_e)}$$

asymmetry — oscillation ratio

Kinematical energy reconstruction

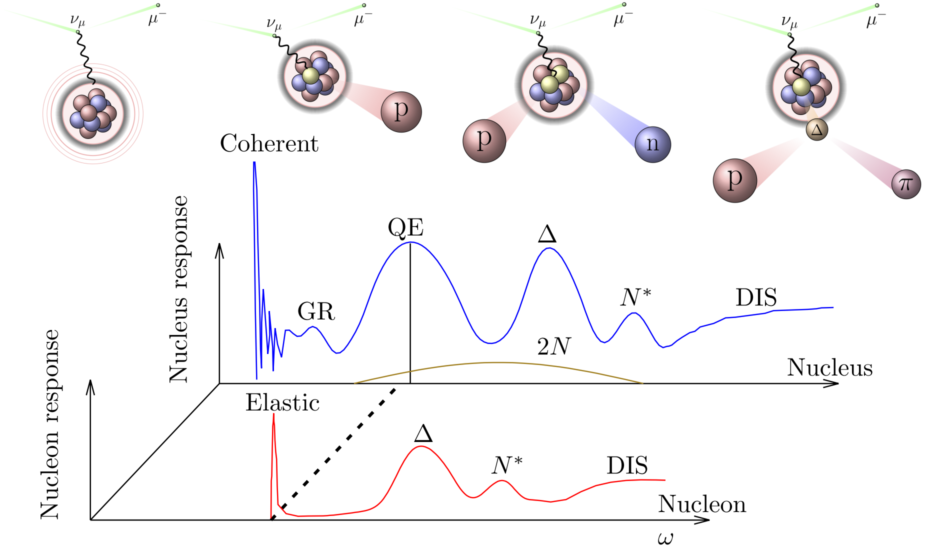
$$E_\nu^{rec} = \frac{2M_N E_\mu - m_\mu{}^2 + M_{N'}^2 - M_N^2}{2(M_N - E_\mu + p_\mu \cos\theta)}$$



$$E_\nu^{rec} = E_\mu - E_B + \sum_{nucl.} T_i + \sum_{mes.} E_j$$

Calorimetric energy reconstruction

Nuclear response

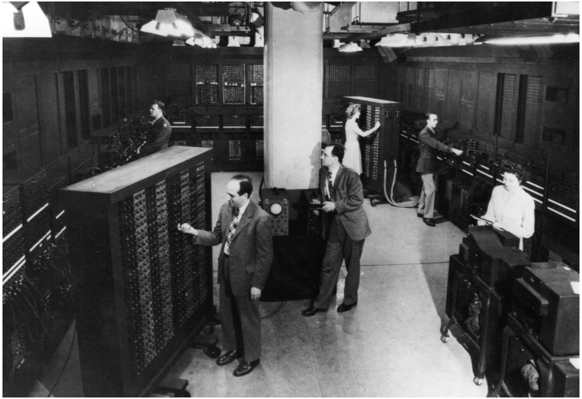


Basic aspects of the methodology

From Solitaire to the Monte Carlo method

At Los Alamos, Stanisław Ulam, John von Neumann, Nicholas Metropolis and others invented a method to obtain stochastic predictions for **systems too complex to be solved analytically**.

- → We can build a complex model using **simple components**
- → Every required decision is **made stochastically** (randomly)
- → We **run** such a model N **times** and analyze the output
- → For $N \to \infty$ we approach the **correct result** for the model



Electronic Numerical Integrator and Computer (ENIAC)

Monte Carlo integration (hit-or-miss method)

Let's consider the **following integral**

$$\int_0^1 f(x)\,dx = \int_0^1 \left(\frac{1}{2}x\right)\,dx = \frac{1}{2}\frac{x^2}{2}\bigg|_0^1 = \frac{1}{4}$$

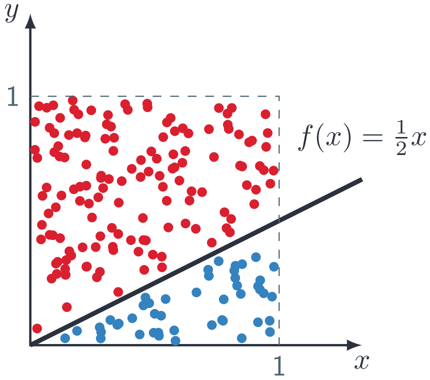
→ Take a random point from $[0;1] \times [0;1]$

→ Compare it to your $f(x)$

→ Repeat N times

→ Count n points below the function

→ The **result is given by** $\int_0^1 f(x)\,dx = A_{\square}\frac{n}{N}$



Monte Carlo integration (crude method)

Let's consider the **following integral** (again)

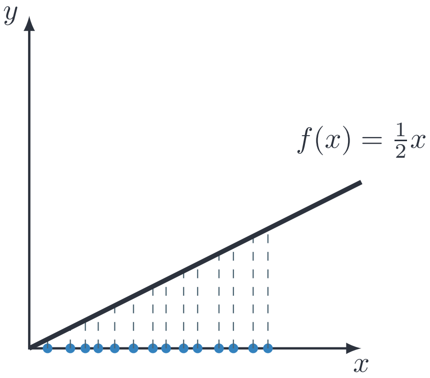
$$\int_0^1 f(x)\, dx = \int_0^1 \left(\frac{1}{2}x\right)\, dx = \frac{1}{2}\frac{x^2}{2}\Big|_0^1 = \frac{1}{4}$$

→ One can **approximate the integral by**

$$\int_a^b f(x)\, dx = \frac{b-a}{N}\sum_i^N f(x_i)$$

where x_i is a random number from $[a; b]$

→ This method leads to slightly higher precision

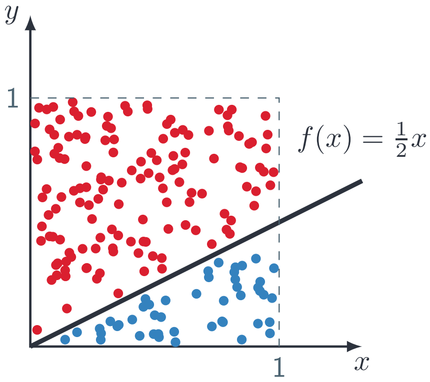


Accept-or-reject algorithm

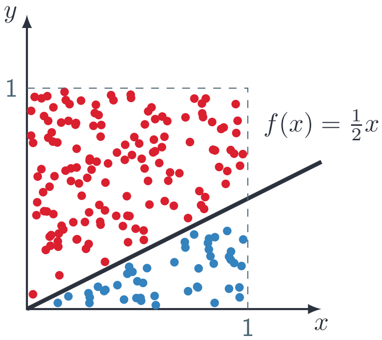
Let's generate a set of points that follows the **probability distribution given by our function**

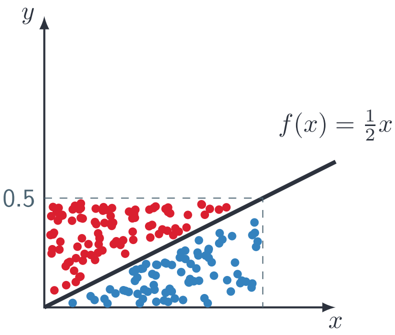
$$f(x) = \frac{1}{2}x$$

- → Find a suitable $f_{max} \geqslant max(f)$
- → Take a **random** x from $[0; 1]$
- → Generate a **random** u from $[0, f_{max}]$
- → **Accept the point** x **if** $u \leqslant f(x)$ $(P = \frac{f(x)}{f_{max}})$



Optimization





→ We wish to **increase the efficiency** of our calculation by avoiding loosing the "red" points

→ We can choose any envelope to our function as long as it **contains the maximum of** $f(x)$

Importance sampling

Let's consider a different function

$$f(x) = A\,x^3\,e^{-x^2}$$

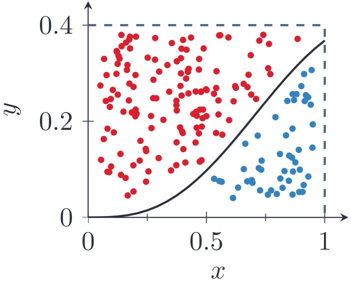
with x in $[0;1]$ and $A = \frac{2e}{e-2}$

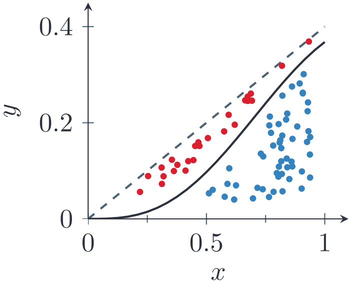
- The area under $f(x)$ is ~ 0.13, while the total is 0.4
- Having a good **x-dep. envelope increases efficiency**

→ For, e.g., $g(x) = 0.4x$, the total area is 0.2

→ We can accept points using a **probability**

$$P(x) = f(x)/g(x)$$





Importance sampling

Let's consider a different function

$$f(x) = A\, x^3\, e^{-x^2}$$

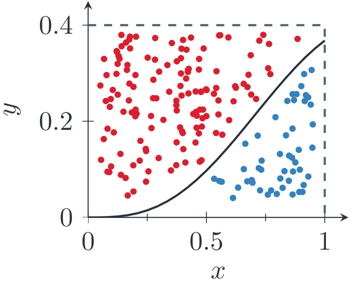
with x in $[0;1]$ and $A = \frac{2e}{e-2}$

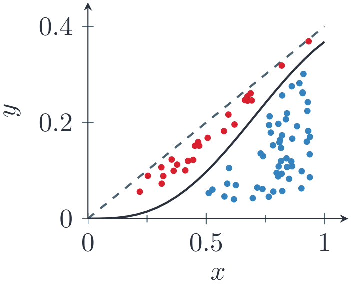
- Alternatively, we could change our random numbers from **non-uniform distributions**

- We can pick more points where the function is larger

→ We can **sample points from** $g(x) = 0.4x$, and correct the probability

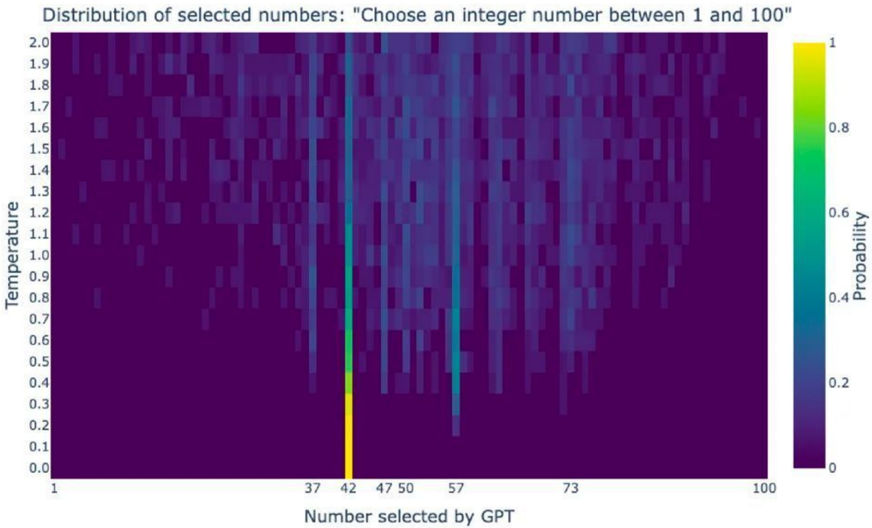
$$\int_0^1 f(x)\, dx \to \int_0^1 \frac{f(x)}{g(x)}\, [g(x)dx]$$





Problems to consider

- How to generate random numbers from a uniform distribution?
- What does it mean for a random number generator to be good?
- How to generate numbers from discrete random variables?
- How to generate numbers from continuous random variables?
- How to generate numbers from arbitrary distributions?



AI Research
by Leniolabs_

Source: ChatGPT prompted 1000 times with
"Choose an integer number between 1 and 100"

Example I: Nucleon propagation

Classical particle propagating through a medium

Probability for a particle to propagate over a distance x with **no interactions** is

$$P(x) = \frac{1}{\lambda}\exp(-x/\lambda)$$

where $\lambda = (\rho\sigma)^{-1}$ is the **mean free path**, while ρ is **target density** and σ is **interaction cross section**

We can try to apply it to nucleons in nuclei because:

$$\tilde{\lambda} \ll d < \lambda < R$$

where $\tilde{\lambda}$ is the de Broglie **wavelength**, d is the **distance** between targets, and R is the **nuclear radius**

N. Metropolis et al., Phys.Rev. 188 (1958) 185, Phys.Rev. 188 (1958) 204

Application to nuclei (space-like approach)

- Pick a random starting point in the nucleus
- Propagate the nucleon in discrete steps, e.g., $\Delta x = 0.2$ fm
- At every step, we sample x from $P(x) = \lambda^{-1} \exp(-x/\lambda)$

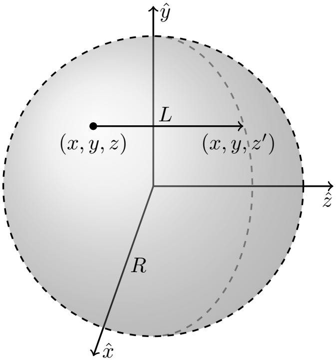
→ If $x < \Delta x$, then the nucleon-nucleon interaction happens

- The probability that the nucleon leaves the nucleus with no re-interactions is called **transparency**

→ Our procedure solves an integral

$$T = \int_0^{2R} f_R(z) e^{-z/\lambda}\, dz$$

where $f_R(z)$ is the distribution of the starting points



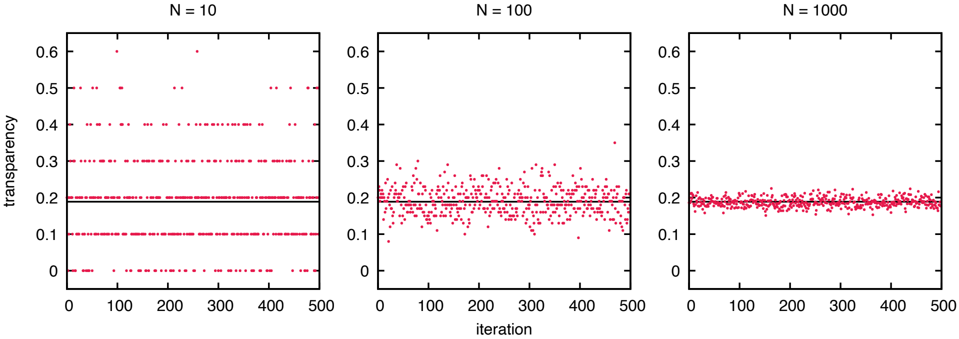
Nuclear transparency

- For fixed density (uniform ball), the **solution is given analytically**

$$T = 3e^{-A}\left(\frac{1}{A^2} + \frac{1}{A^3}\right) + 3\left(\frac{1}{2A} - \frac{1}{A^3}\right)$$

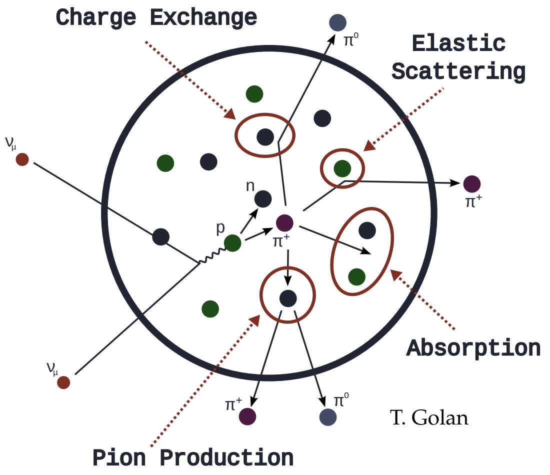
where $A = 2R/\lambda = 2R\rho\sigma$

→ e.g., for $\rho = 0.16\ \mathrm{fm}^{-3}$, $\sigma = 40$ mb, and $R = 6$ fm, we get $T \simeq 0.189$



Intranuclear cascade

- → implement **realistic density profiles** and **cross sections**
- → add the **kinematics** of each interaction
- → respect **Pauli blocking**
- → make sure that **scattered particles also propagate**
- → introduce **branching ratios** of different channels
- → track also **other hadrons**
- → add **other nuclear effects**...



Lepton-nucleus scattering

General remarks

- Leptons are **Standard Model particles**

→ there are better ways to model their interactions than billiard balls

- Lepton-nucleon **cross section is lower** than nucleon-nucleon

→ we do not shoot at nuclei, we start from the primary interaction

→ we need an external lepton-nucleus cross section model

- Lepton-nucleus interactions **require great precision**

→ common detector simulation software do not contain these processes

Independent variables

Unknown particle 4-vectors	Variables	Physical effects	Variables
Initial lepton	4	Particles on-shell	$-(3+N)$
Target nucleus	4	4-momentum conservation	-4
Final lepton	4	Target rest-frame	-3
Remnant nucleus	4	Fixed projectile direction	-2
Outgoing hadrons	$4N$	Fixed incoming energy	-1
	$16+4N$		$-13-N$
			$3+3N$

Table 1.2: Counting the number of independent variables describing lepton-nucleus interactions while detecting N hadronic particles in the process, summing over the spin of the outgoing lepton, and leaving the remnant nucleus undetected.

Cross sections

Target	Process	Properties	Example formula
Free nucleon	(Quasi)elastic	$N = 0$, all particles on-shell	$\frac{d\sigma}{dQ^2}$
	Inelastic	$N = 0$, excited hadronic system	$\frac{d^2\sigma}{dQ^2 dW}$
	SPP	$N = 1$, all particles on-shell	$\frac{d^4\sigma}{dQ^2 dW d\Omega_\pi}$
Nucleus	Inclusive	$N = 0$, all hadrons integrated	$\frac{d^2\sigma}{d\Omega'}$
	1p1h	$N = 1$, detected one nucleon	$\frac{d^5\sigma}{dE' d\Omega' d\Omega_{N'}}$
	2p2h	$N = 2$, detected two nucleons	$\frac{d^8\sigma}{dE' d\Omega' dE_{N'} d\Omega_{N'} d\Omega_{N''}}$
	SPP	$N = 2$, detected nucleon and π	$\frac{d^8\sigma}{dE' d\Omega' dE_\pi d\Omega_\pi d\Omega_{N'}}$

Table 1.3: The dimensionality of cross section formulas for the most basic lepton scattering scenarios, off the free nucleon or on the nucleus.

Example II: Quasielastic neutrino-nucleon scattering

Quasielastic scattering on a free nucleon

Llewellyn-Smith formula

$$\frac{d\sigma}{d|q^2|}\begin{pmatrix}\nu_l + n \to l^- + p \\ \bar{\nu}_l + p \to l^+ + n\end{pmatrix} = \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2}\left[A(q^2) \mp B(q^2)\frac{(s-u)}{M^2} + C(q^2)\frac{(s-u)^2}{M^4}\right]$$

Notation

- constants: M - nucleon mass, G_F - Fermi constant, θ_C - Cabbibo angle
- $q^2 = (k-k')^2 = (p'-p)^2$ - four-momentum squared, where k, k', p, p' are four-momenta of initial and final lepton, initial and final nucleon
- E_ν - neutrino energy
- $s = (k+k')^2$ and $u = (k-p')^2$ - Mandelstam variables

Quasielastic scattering on a free nucleon

Llewellyn-Smith formula

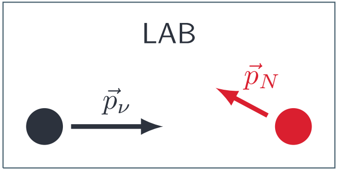
$$\frac{d\sigma}{d|q^2|}\begin{pmatrix}\nu_l + n \to l^- + p \\ \bar{\nu}_l + p \to l^+ + n\end{pmatrix} = \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2}\left[A(q^2) \mp B(q^2)\frac{(s-u)}{M^2} + C(q^2)\frac{(s-u)^2}{M^4}\right]$$

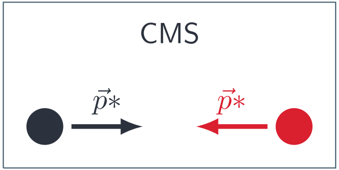
General idea

- having k and p, generate k' and p'
- calculate q^2 and $(s-u) = 4ME_\nu + q^2 - m^2$ based on the generated kinematics
- calculate the cross section
- repeat N times and the result is given by

$$\sigma_{\text{total}} \sim \frac{1}{N}\sum_i^N \sigma(q_i^2)$$

Generating kinematics





- Let's consider kinematics in the center-of-mass system
- Mandelstam s is invariant under Lorentz transformation

$$s = (k + p)^2 = (E + E_p)^2 - (\vec{k} + \vec{p})^2 = (E^* + E_p^*)^2$$

- $\sqrt{s}$ is the total energy in CMS

$$\sqrt{s} = E^* + E_p^* = \sqrt{p^{*2} + m^2} + \sqrt{p^{*2} + M^2}$$

- We will use it to calculate p^*

Generating kinematics

- After some simple algebra

$$
\begin{aligned}
\sqrt{s} &= E^* + E_p^* = \sqrt{p^{*2} + m^2} + \sqrt{p^{*2} + M^2} \\
\sqrt{s} &= E^* + \sqrt{E^{*2} - m^2 + M^2} \\
s &= E^{*2} + E^{*2} - m^2 + M^2 + 2E^* E_p^* \\
s &= 2E^*(E^* + E_p^*) - m^2 + M^2 \\
s &= 2E^* \sqrt{s} - m^2 + M^2
\end{aligned}
$$

and

$$
\begin{aligned}
E^* &= \frac{s + m^2 - M^2}{2\sqrt{s}} \\
E_p^* &= \frac{s + M^2 - m^2}{2\sqrt{s}}
\end{aligned}
$$

- We use this result to get

$$
p^* = \sqrt{E^{*2} - m^2} = \frac{[s - (m - M)^2][s - (m + M)^2]}{2\sqrt{2}}
$$

Generating events

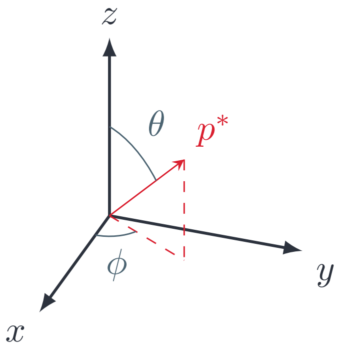
- We use spherical coordinate system to determine momentum direction in CMS

$$\vec{p}^* = p^* \cdot (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$$

- Generating random angles

$$\begin{aligned} \phi^* &= 2\pi \cdot \text{random}[0;1] &\rightarrow\ & \sin\phi^*, \cos\phi^* \\ \cos\theta^* &= 2 \cdot \text{random}[0;1] - 1 &\rightarrow\ & \sin\phi^*, \cos\phi^* \end{aligned}$$

- Now, we need to come back to the LAB frame



Boosting between frames

- Lorentz boost in the direction $\hat{n} = \frac{\vec{v}}{v}$ of $(t, \vec{r})$

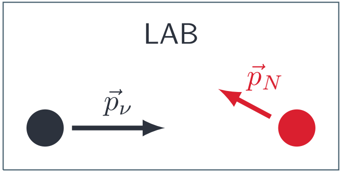
$$
\begin{aligned}
t' &= \gamma(t - v\hat{n}\cdot\vec{r}) \\
r' &= \vec{r} + (\gamma - 1)(\hat{n}\cdot\vec{r})\hat{n} - \gamma t v \hat{n}
\end{aligned}
$$

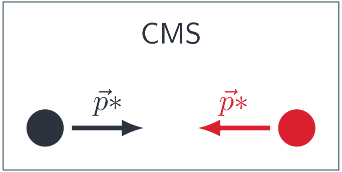
- In our case

$$\vec{v} = \frac{\vec{p}_\nu + \vec{p}_N}{E_\nu + E_N}$$

- Boost from LAB to CMS in the $\vec{v}$ direction

- Boost from CMS to LAB in the $-\vec{v}$ direction





Calculating the cross section

Llewellyn-Smith formula

$$\frac{d\sigma}{d|q^2|}\begin{pmatrix}\nu_l + n \to l^- + p \\ \bar{\nu}_l + p \to l^+ + n\end{pmatrix} = \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2}\left[A(q^2) \mp B(q^2)\frac{(s-u)}{M^2} + C(q^2)\frac{(s-u)^2}{M^4}\right]$$

Calculation

- once we have p', k' in the LAB frame, we can calculate q^2 ans $(s-u)$
- once we have q^2, we can calculate $A(q^2)$, $B(q^2)$, and $C(q^2)$
- we have all we need to calculate the final result

$\rightarrow$ but we changed variables so we need a Jacobian!

Calculating the cross section

- Express q^2 in terms of the lepton angle (in CMS)

$$q^2 = (k - k')^2 = (k^* - k'^*)^2 = m^2 - 2k^* \cdot k'^* = m^2 = 2EE' + 2|\vec{k}^*||\vec{k}'^*| \cos\theta^*$$

- Thus, the Jacobian is given by

$$dq^2 = 2|\vec{k}^*||\vec{k}'^*| \, d\cos\theta^*$$

- The total cross section is given by

$$\sigma = \int_{-1}^{1} \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2} \left[A(q^2) \mp B(q^2) \frac{(s-u)}{M^2} + C(q^2) \frac{(s-u)^2}{M^4} \right] 2|\vec{k}^*||\vec{k}'^*| \, d\cos\theta^*$$

$$\sigma_{MC} = \frac{2}{N} \sum_i^N \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2} \left[A(q^2) \mp B(q^2) \frac{(s-u)}{M^2} + C(q^2) \frac{(s-u)^2}{M^4} \right] 2|\vec{k}^*||\vec{k}'^*|$$

Calculating the cross section

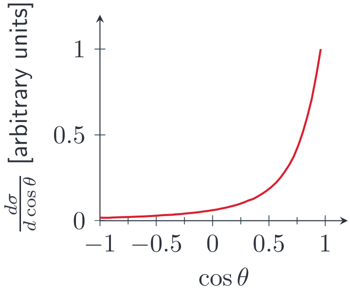
- We want to avoid any sharp peaks as they affect our efficiency and accuracy

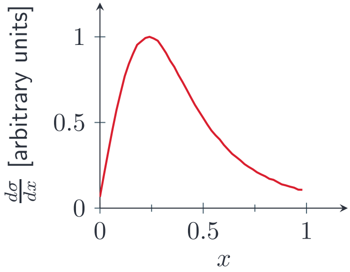
- Let's change the variable once again

$$\cos\theta^* = 1 - 2x^2, \; x \in [0; 1]$$

- Notice, the new Jacobian and integration limits

$$2\int_{-1}^{1} \mathrm{d}\cos\theta^* \;\rightarrow\; \int_{1}^{0} \mathrm{d}x\,(-4x) \;\rightarrow\; \int_{0}^{1} 4x\,\mathrm{d}x$$





Calculating the cross section

- Finally, the total cross section is given by

$$\sigma = \int_{-1}^{1} \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2} \left[A(q^2) \mp B(q^2) \frac{(s-u)}{M^2} + C(q^2) \frac{(s-u)^2}{M^4} \right] 2|\vec{k}^*||\vec{k}'^*| 4x \, dx$$

$$\sigma_{MC} = \frac{1}{N} \sum_i^N \frac{M^2 G_F^2 \cos\theta_C}{8\pi E_\nu^2} \left[A(q^2) \mp B(q^2) \frac{(s-u)}{M^2} + C(q^2) \frac{(s-u)^2}{M^4} \right] 2|\vec{k}^*||\vec{k}'^*| 4x$$

- In conclusion: do some kinematics, add some boosts between CMS and LAB, change the integration variable several times... and you are ready to calculate the cross section

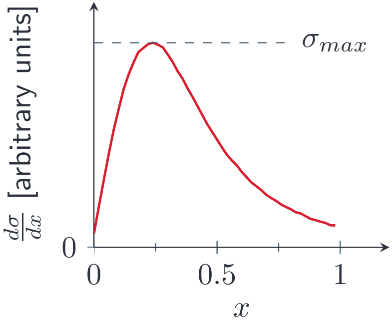
→ Now, we need to generate some events that are distributed according to the cross section formula

Generating events

- Take a random x from $[0; 1]$
- Do the kinematics

$$\begin{aligned} x &\rightarrow \cos\theta^* \\ \cos\theta^* &\rightarrow k'^*, p'^* \\ k'^*, p'^* &\rightarrow k', p' \\ &\ldots \end{aligned}$$

- Calculate the cross section
- Accept an event with the probability $P(x) = \frac{\sigma(x)}{\sigma_{\text{max}}}$



Are we there yet?

A few more steps...

→ add **other dynamics**: single-pion production, deep inelastic scattering...

→ add support for **nuclei** as **targets**

→ if you have a nucleus, add some **two-body current interactions**

→ if you have a nucleus, add some nuclear effects: **Pauli blocking**, **final-state interactions**...

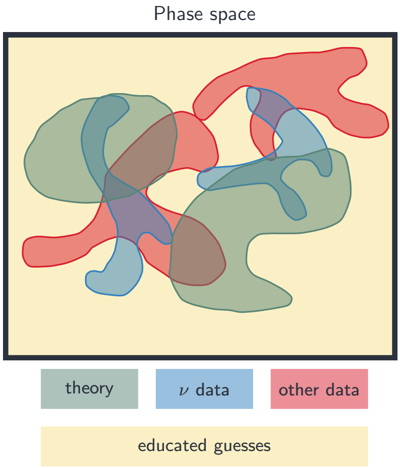
→ add support for **neutrino beams**

→ add support for **detector geometries**

→ add some **reweighting**

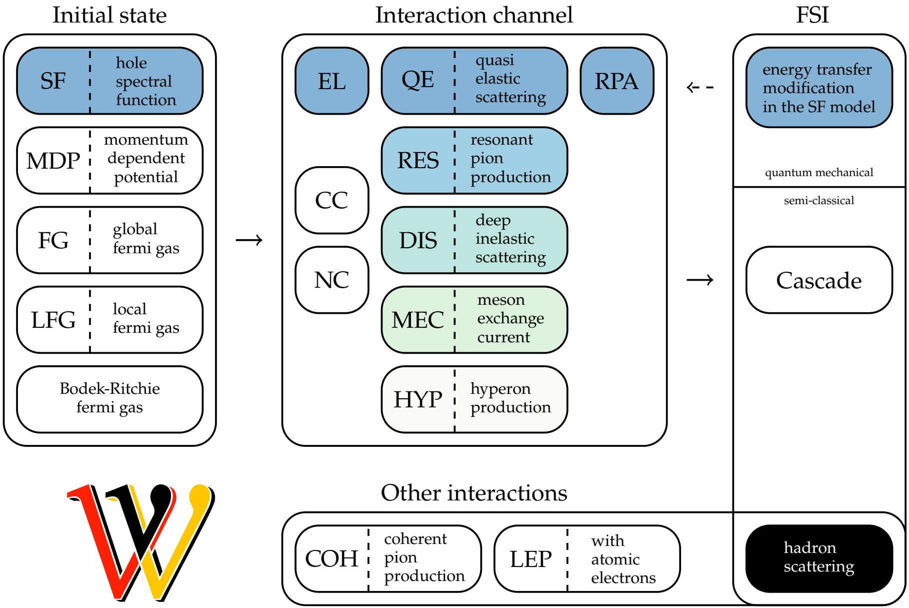
... and your MC generator is done!

Ingredients



Recipe

NuWro
Monte Carlo event generator



Supplementary material

MC integration (hit-or-miss method)

Let's consider the following integral

$$\int_0^1 f(x)dx = \int_0^1 \left(\frac{1}{2}x\right) dx = \frac{1}{2}\frac{x^2}{2}\bigg|_0^1 = \frac{1}{4}$$

→ take a random point from a $[0,1] \times [0,1]$ square

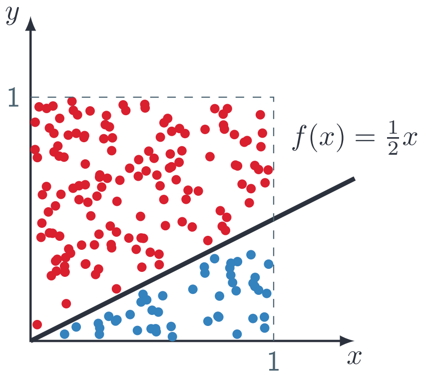
→ compare it to your $f(x)$

→ repeat N times

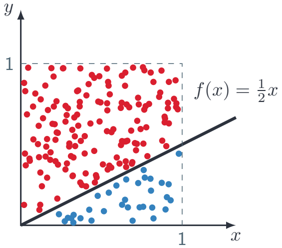
→ count n points below the function

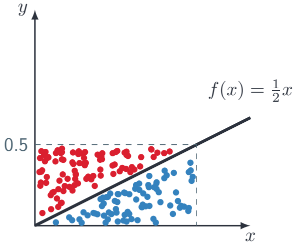
→ your result is given by

$$\int_0^1 f(x)dx = A_{\Box} \cdot \frac{n}{N}$$



Optimizations





- We want to **avoid** generating "**red**" points as they do not contribute to your integral
- **Any rectangle** can be chosen as far as it **contains maximum** of $f(x)$ in given range

Optimizations

- Consider the following function

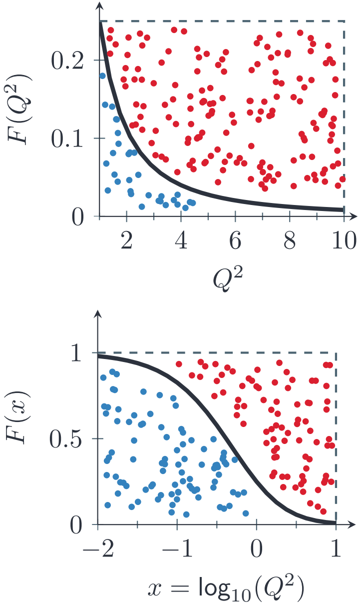
$$F(Q^2) = \frac{1}{(1+Q^2)^2}$$

- Integrating this function over Q^2 is highly inefficient

- One can integrate by substitution to get better performance, e.g.

$$x = \log_{10} Q^2$$

→ don't forget about the Jacobian!



MC integration (crude method)

Let's consider the following integral again

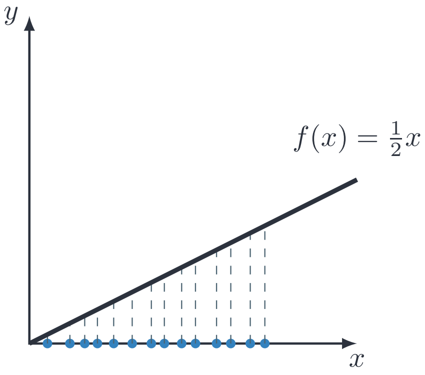
$$\int_0^1 f(x)dx = \int_0^1 \left(\frac{1}{2}x\right) dx = \frac{1}{2}\frac{x^2}{2}\Big|_0^1 = \frac{1}{4}$$

- One can approximate the integral

$$\int_a^b f(x)dx = \frac{b-a}{N}\sum_i^N f(x_i)$$

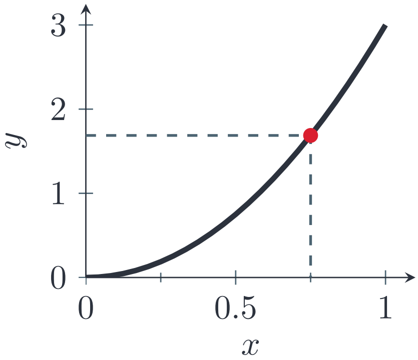
  where x_i is a random number from $[a, b]$

- It can be shown that this method is more accurate



Random numbers from probability density functions

- How to generate a random number from probability density function?
- Let's consider $f(x) = 3x^2$
- Which means that $x = 1$ should be thrown 2 times more often than $x = \frac{\sqrt{2}}{2}$



Cumulative distribution function

- Cumulative distribution function of a random variable X:

$$F(x) = P(X \leq x)$$

- Discrete random variable X:

$$F(x) = \sum_{x_i \leq x} f(x_i)$$

where f is a probability mass function (PMF)

- Continuous random variable X:

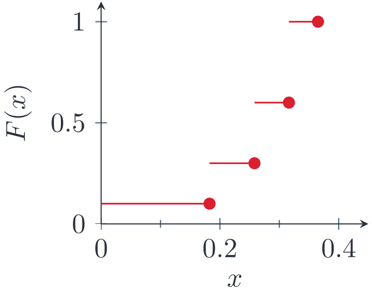
$$F(x) = \int_{-\infty}^{x} f(t)\mathrm{d}t$$

where f is a probability density function (PDF)

Cumulative distribution function - discrete example

- Probability mass function $f(x) = 3x^2$
  with discrete random variables X is $\{\sqrt{\frac{1}{30}}, \sqrt{\frac{2}{30}}, \sqrt{\frac{3}{30}}, \sqrt{\frac{4}{30}}\}$
- CDF is given by

$$F(x) = \begin{cases} \frac{1}{10} & \text{if } x \leq \sqrt{\frac{1}{30}} \\ \frac{3}{10} & \text{if } x \leq \sqrt{\frac{2}{30}} \\ \frac{6}{10} & \text{if } x \leq \sqrt{\frac{3}{30}} \\ \frac{10}{10} & \text{if } x \leq \sqrt{\frac{4}{30}} \end{cases}$$



$\rightarrow$ generate a random number u from $[0, 1]$

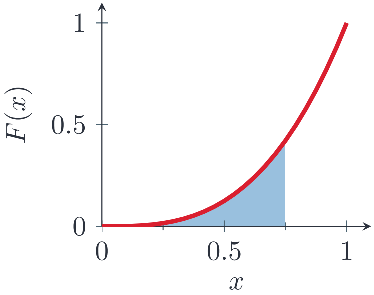
$\rightarrow$ if $u \leq 0.1$: $x = \sqrt{\frac{1}{30}}$ $\quad\rightarrow$ else if $u \leq 0.3$: $x = \sqrt{\frac{2}{30}}$...

Cumulative distribution function - continuous example

- Probability density function $f(x) = 3x^2$
  with continuous random variables X range $[0, 1]$

- CDF is given by

$$F(x) = \int_0^x f(t)\mathrm{d}t = x^3$$



→ generate a random number u from $[0, 1]$

→ find x for which $F(x) = u$, i.e. $x = F^{-1}(u)$

- Unfortunately, usually F^{-1} is unknown, which makes this method pretty useless (at least directly)

Acceptance-rejection method

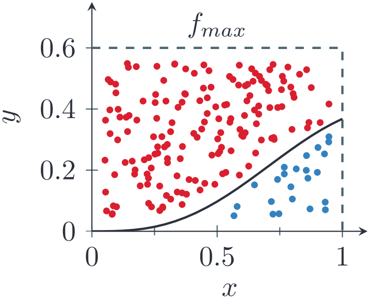
- Let's consider a function $f(x) = A \cdot x^3 \cdot e^{-x^2}$ with $x \in [0, 1]$, $A = \frac{2e}{e-2}$
- CDF is given by $F(x) = \frac{N}{2}(x^2 - 1)e^{-x^2}$ and we don't know F^{-1}!

→ find a suitable $f_{\mathrm{max}} \geq max(f)$

→ take a random x

→ generate a random u from $[0, f_{\mathrm{max}}]$

→ accept if $u \leq f(x)$ ($P = \frac{f(x)}{f_{\mathrm{max}}}$)



- The same procedure as the integration via hit-or-miss but focusing on accepted points, not the integral itself

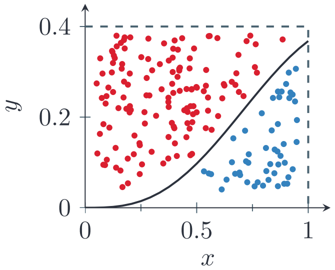
Acceptance-rejection method - optimization

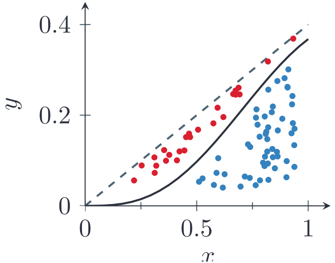
- The area under the plot of $f(x)$ is ~ 0.13, while the total area is 0.4
- We can try to limit the number of wasted points taking a better envelope
- For $g(x) = 0.4x$ the total area is 0.2, so we speed up twice

→ The culumative distribution is $G(x) = x^2$, $G^{-1}(x) = \sqrt{x}$

→ Generate a random $u \in [0, 1]$

→ Calculate $x = G^{-1}(u)$ and accept with probability $P = f(x)/g(x)$





Importance sampling

- Sampling more significant parts of phase space more often

$$\int_0^1 f(x)\mathrm{d}x$$

$$\to \int_0^1 \frac{f(x)}{g(x)}[g(x)\mathrm{d}x]$$

- Mathematically speaking all three methods are equivalent