Monte Carlo basics
I

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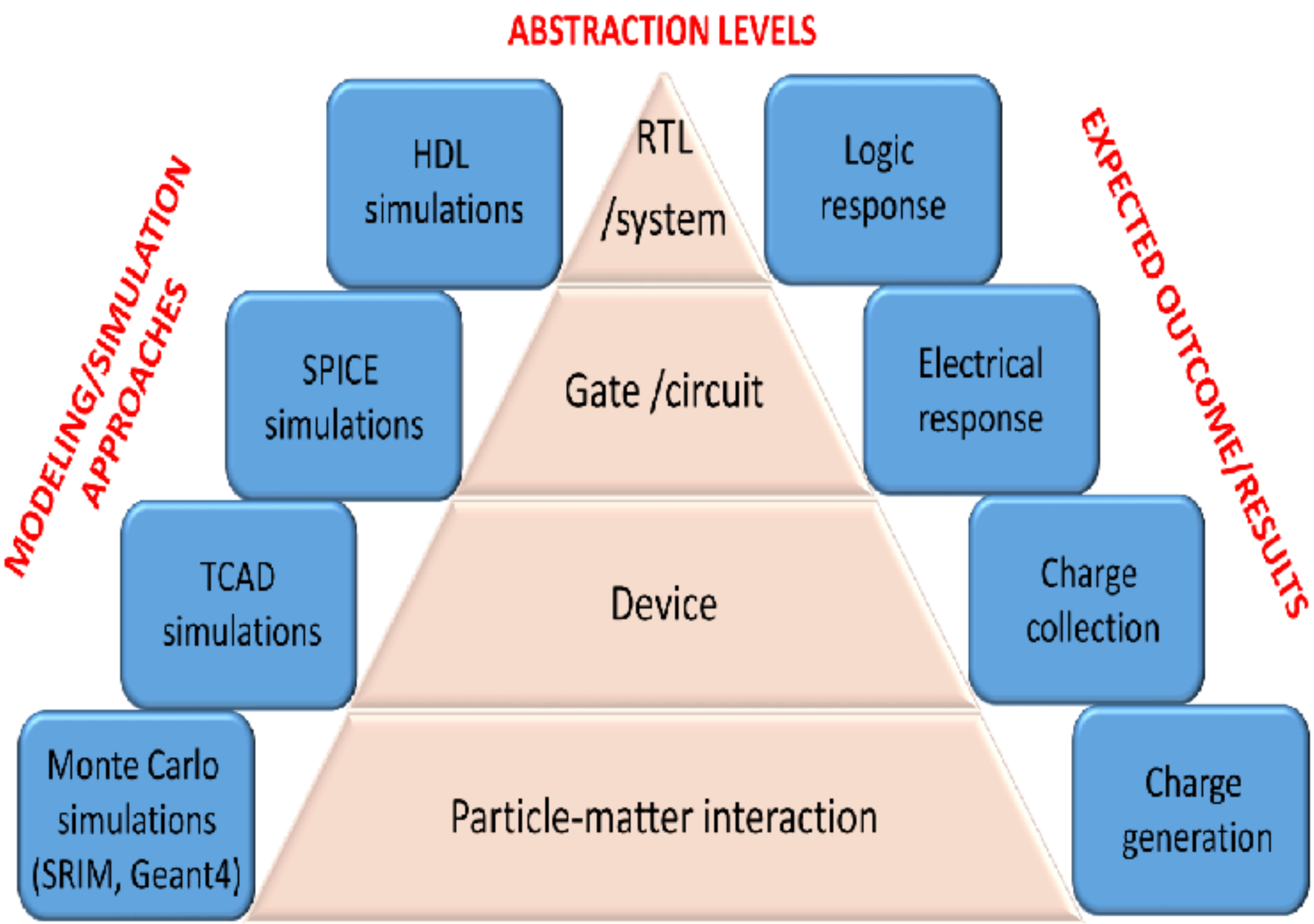
UNIVERSIDAD DE GRANADA

Milos Krstic presentation
Online ELICSIR Summer School
Radiation Effects in Electronic Devices, Circuits and Systems
26/07/2020

Multi-level SEE Modeling and Simulation



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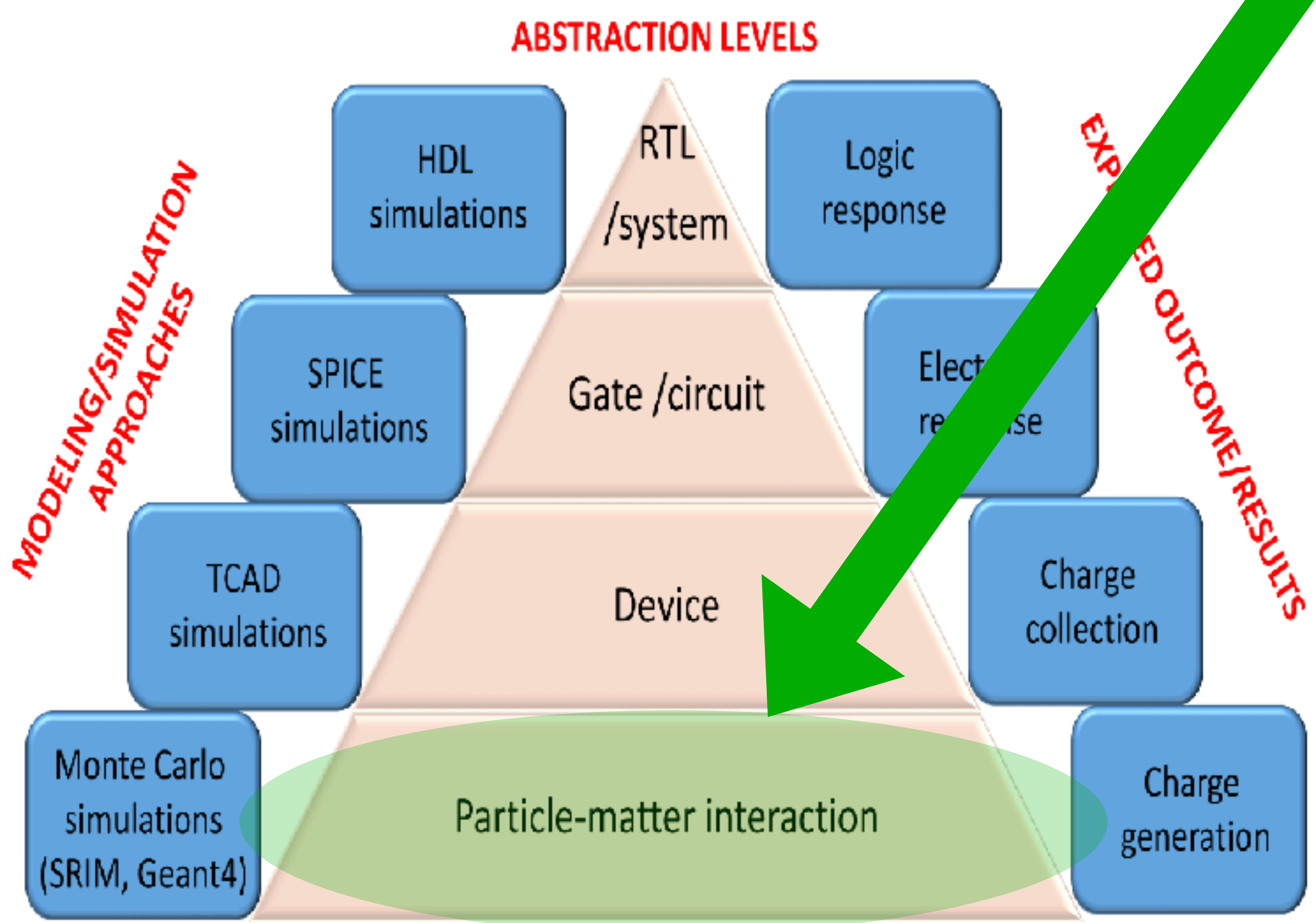

Low statistics problems

MOSFET used as dosimeters

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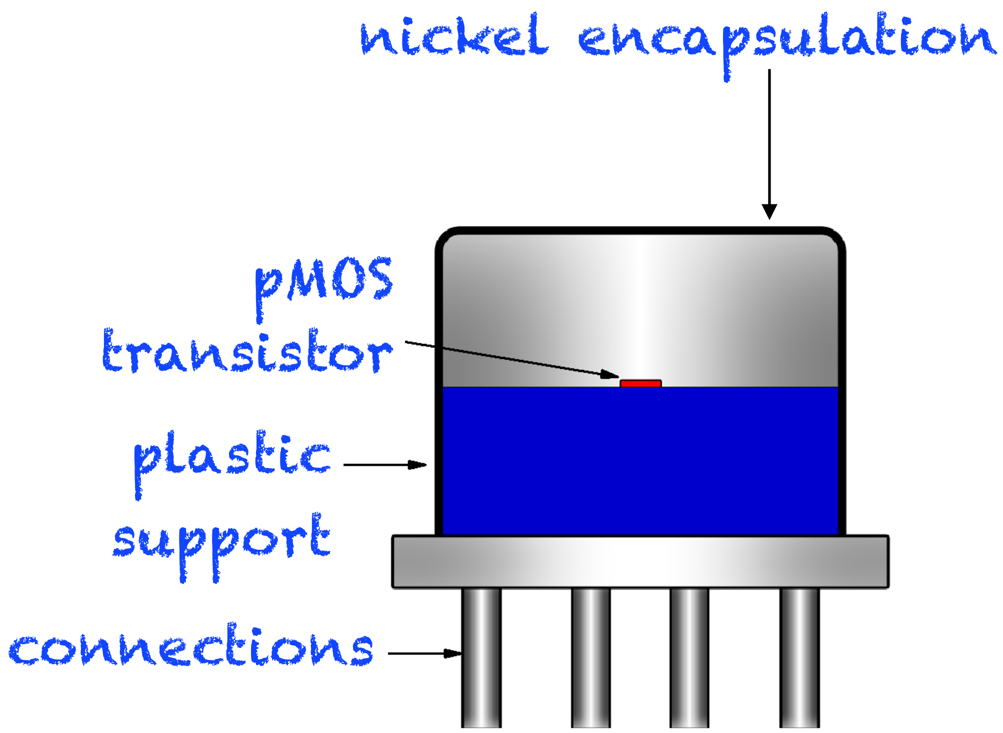

-detector dimensions:
0.42 x 0.49 x 0.1 mm^3

Low statistics problems

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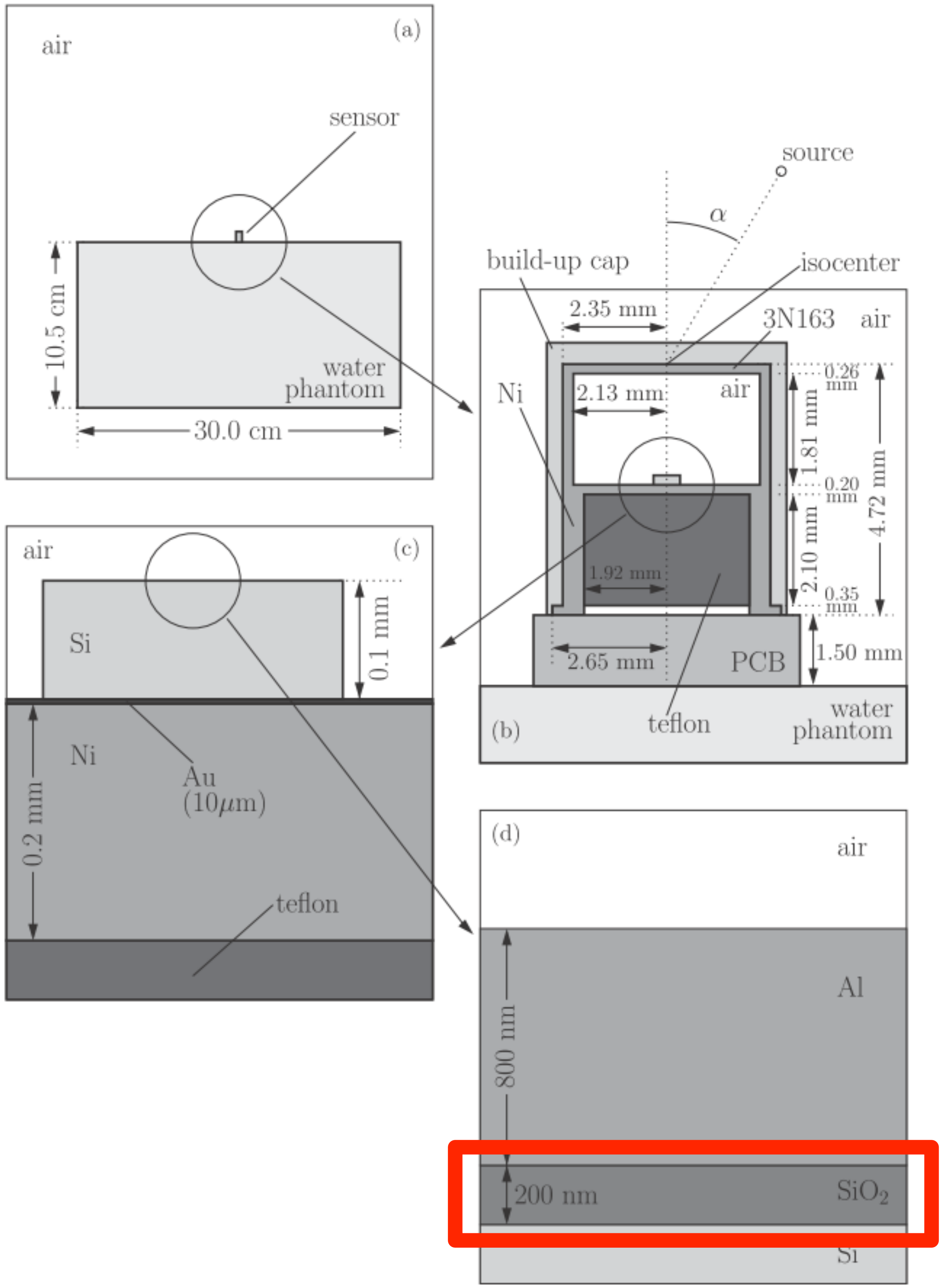

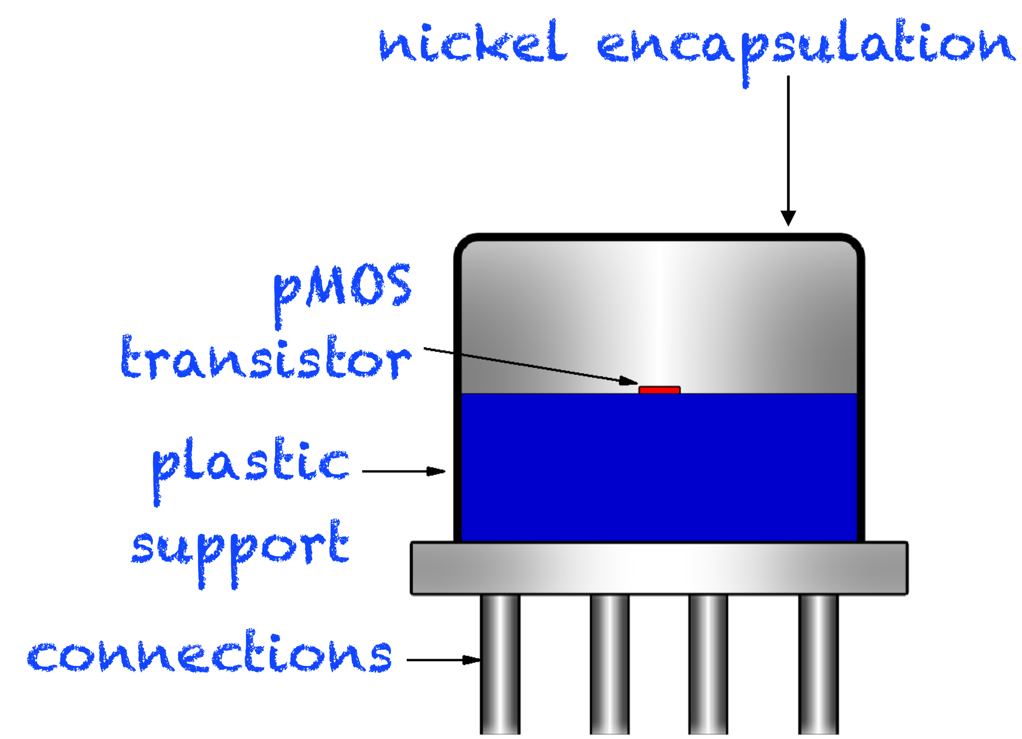

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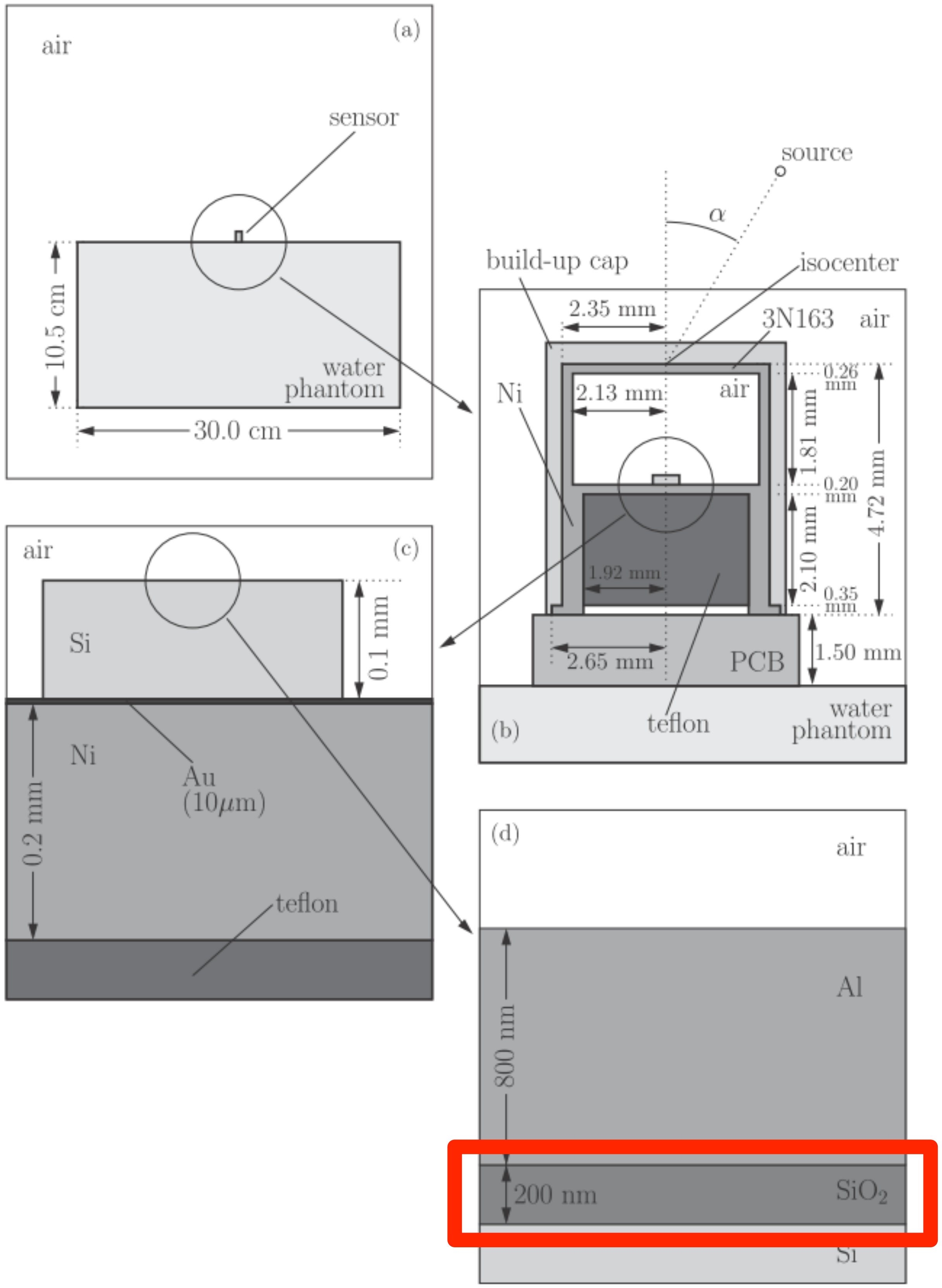

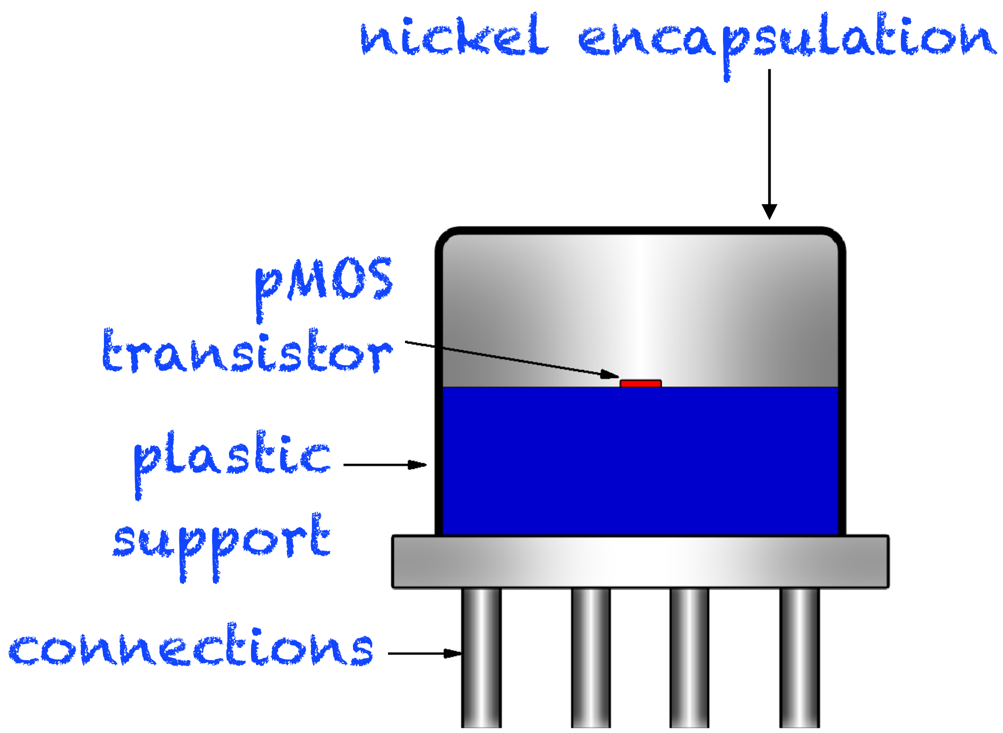

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$0.42 \times 0.49 \times 0.1\ mm^3$

-MOSFET response:
energy deposited in the SiO_2 die

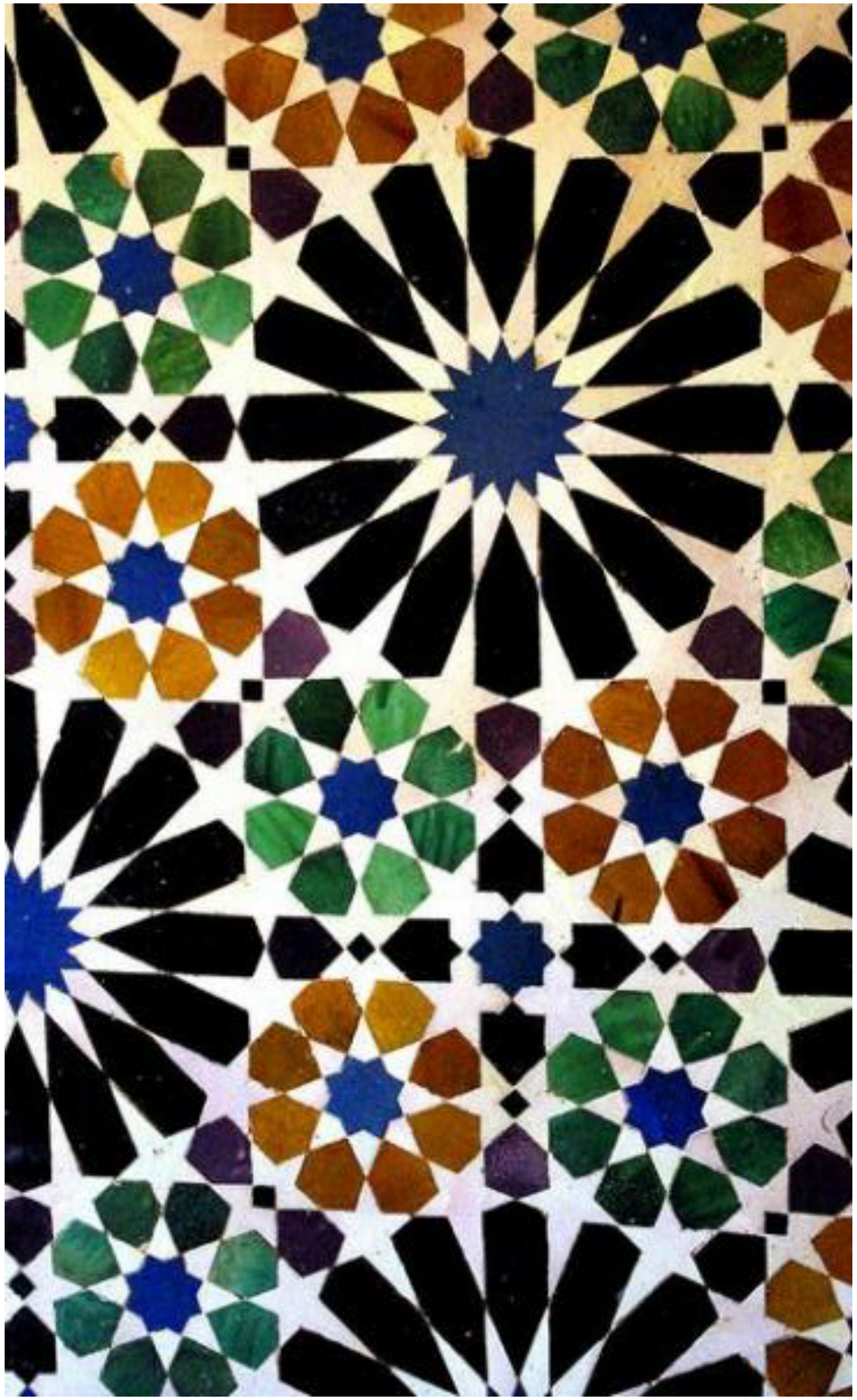
-very low statistics: 30 days for an uncertainty of 10% (k=3)
[Intel Hapertown E5405 2.0 GHz]

Outline

- Monte Carlo simulation of radiation-matter interaction

- Sampling distributions

- Some simple exercises



- Monte Carlo techniques:
  procedures using random numbers to solve problems

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  simulation of stochastic systems

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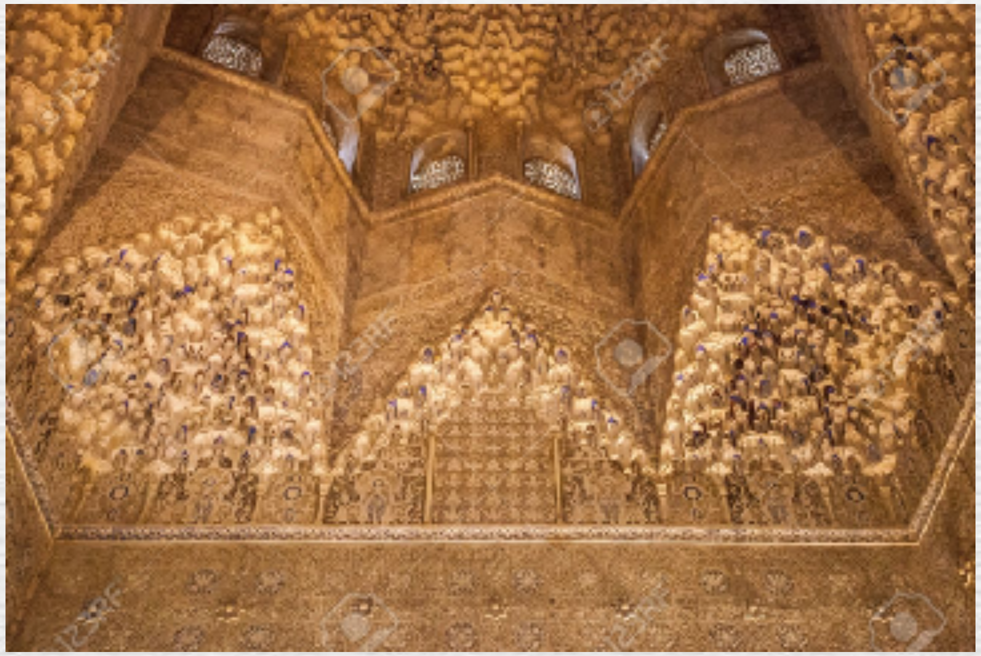
- problems in which chance is essential:
  <u>simulation</u> of stochastic systems

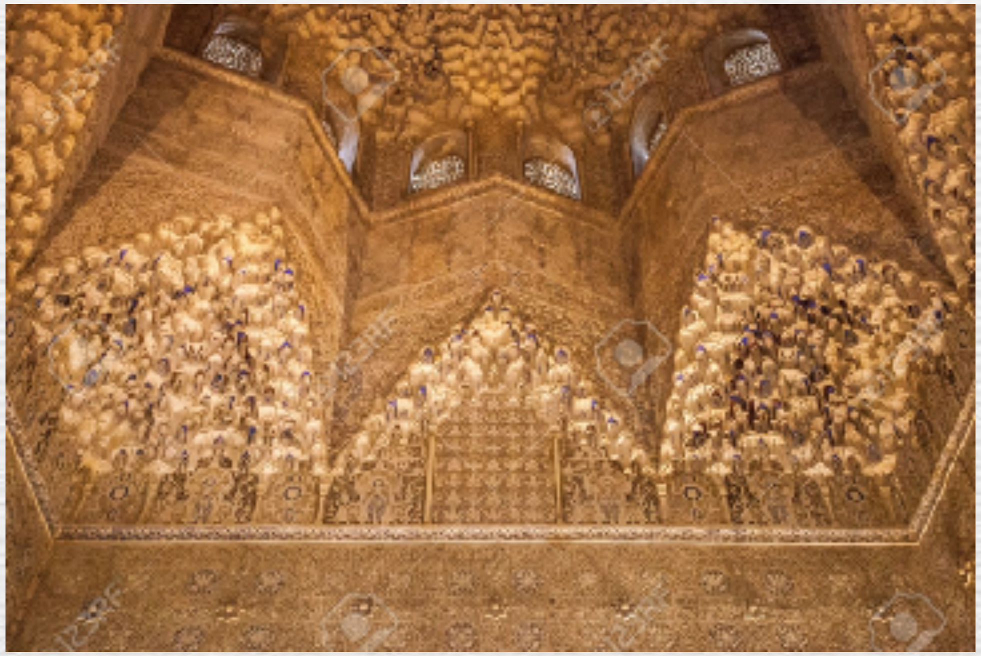
- deterministic calculations reformulated in
  terms of probability distributions:
  calculation of integrals

MC simulation of radiation-matter interaction



MC simulation of radiation-matter interaction

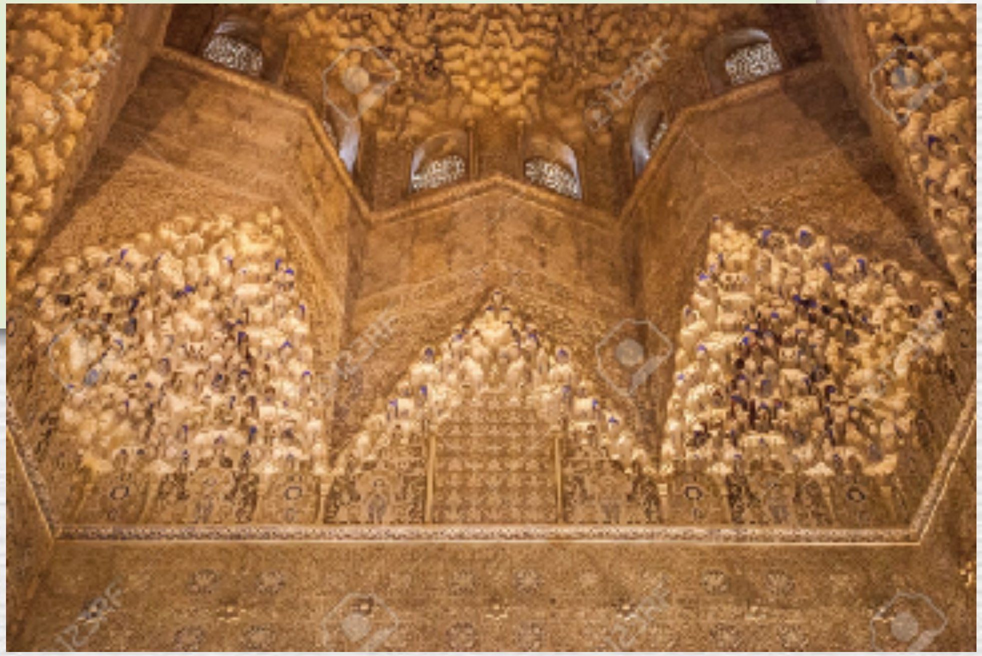
a tool of interest in many fields:



MC simulation of radiation-matter interaction

a tool of interest in many fields:

- ➡electron/positron surface spectroscopy
- ➡electron microscopy
- ➡microanalysis with electron probe
- ➡design and use of radiation detectors
- ➡dosimetry
- ➡radiotherapy
- ➡etc.



what are we trying to simulate?

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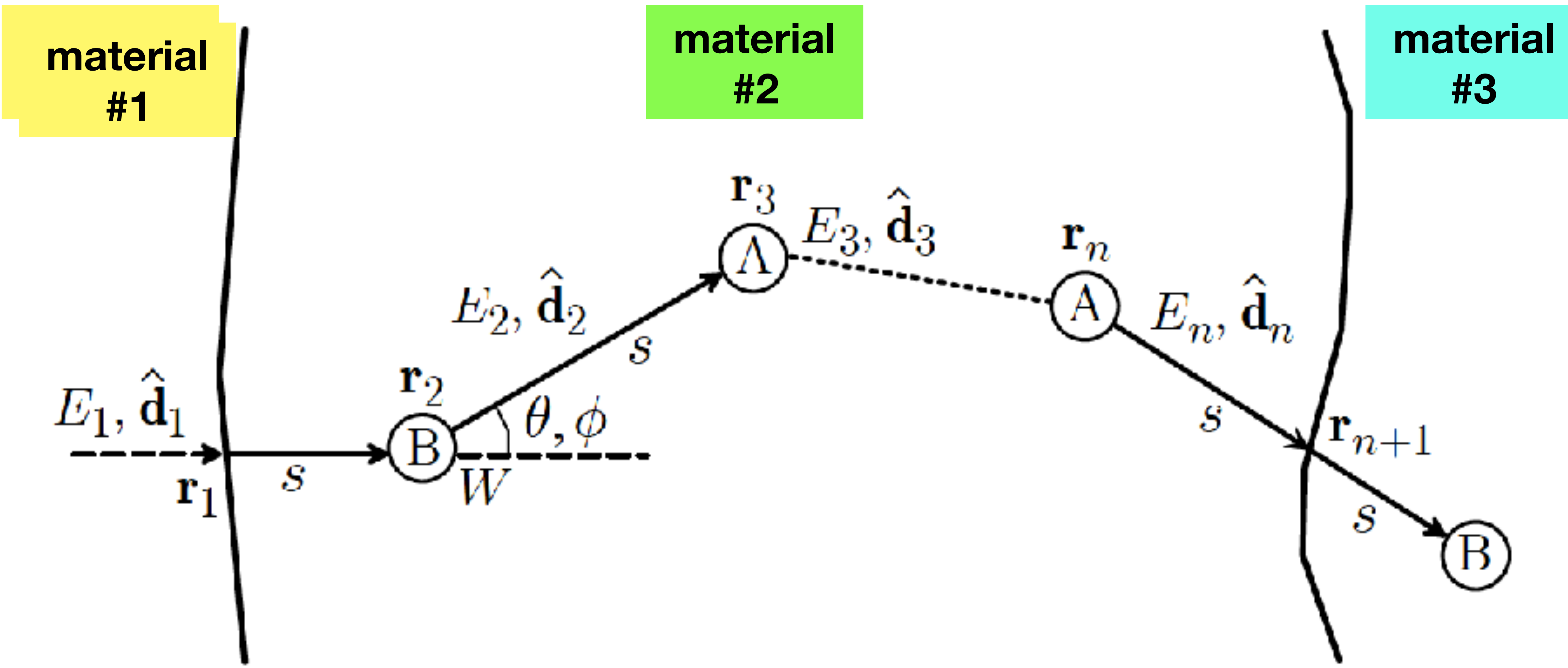

MC simulation of radiation-matter interaction

which material media are we interested in?

MC simulation of radiation-matter interaction

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homogeneous materials with uniform density

MC simulation of radiation-matter interaction

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homogeneous materials with uniform density

- gases, liquids or amorphous solids
- particles are scattered randomly
- molecular weight: $A_{\mathrm{M}} = \sum_i n_i A_i$
- number of molecules per unit volume in the material: $\mathcal{N} = N_{\mathrm{A}} \dfrac{\rho}{A_{\mathrm{M}}}$

MC simulation of radiation-matter interaction

- let us assume a particle moving inside a medium

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- let us assume that the particle interacts with the medium molecules via two mechanisms:
  - A and B
  - no secondary particle production

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-scattering model:

$$\frac{\mathrm{d}^2\sigma_\alpha}{\mathrm{d}W\mathrm{d}\Omega}(E;W,\theta) \qquad \alpha = A,B$$

$W \equiv$ energy loss after the interaction

$\Omega \equiv$ solid angle in the new direction

MC simulation of radiation-matter interaction

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-partial cross sections:

$$\sigma_\alpha(E) \;=\; 2\pi \int_0^E \mathrm{d}W \int_0^\pi \mathrm{d}\theta\,\sin\theta\,\frac{\mathrm{d}^2\sigma_\alpha}{\mathrm{d}W\,\mathrm{d}\Omega}(E;W,\theta)$$

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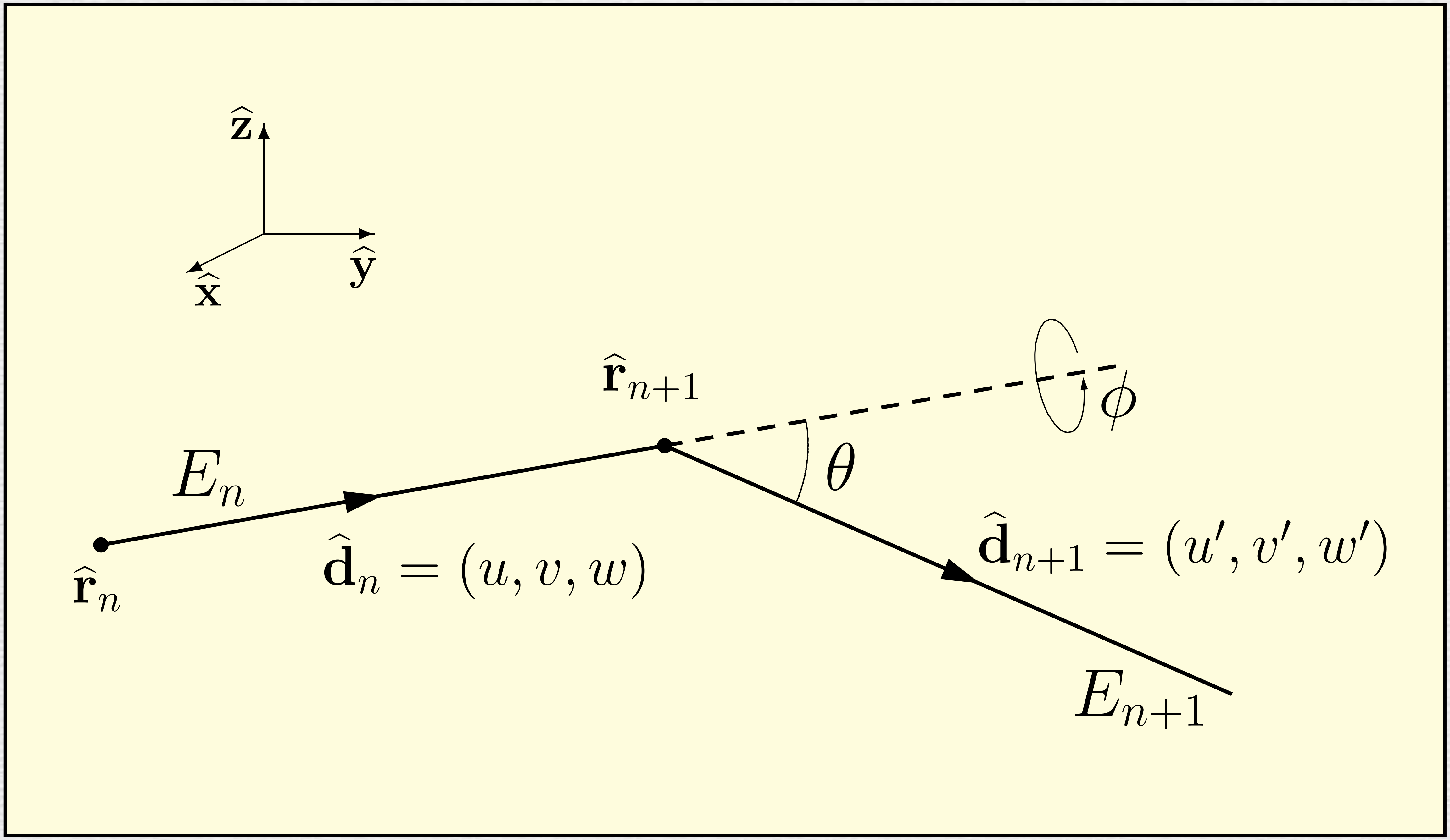
-total scattering cross section:

$$\sigma_\mathrm{T}(E) \;=\; \sum_{\alpha\equiv\,\text{A,B}} \sigma_\alpha(E)$$

MC simulation of radiation-matter interaction



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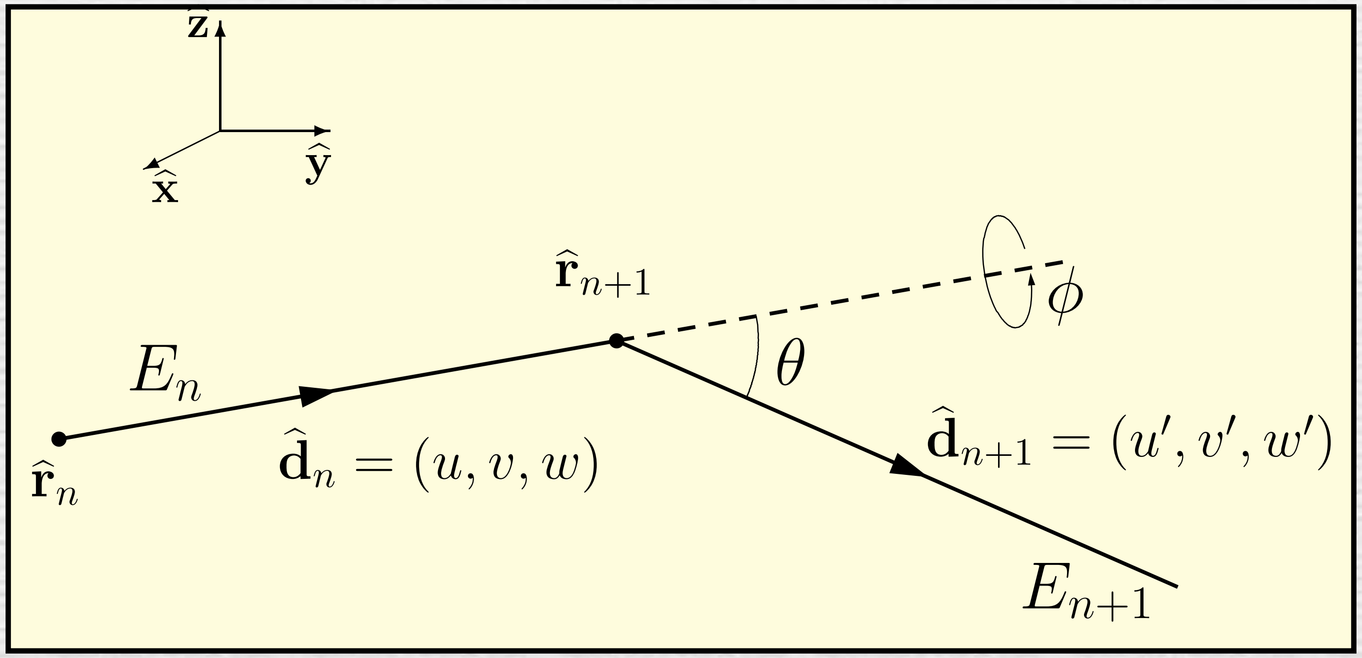

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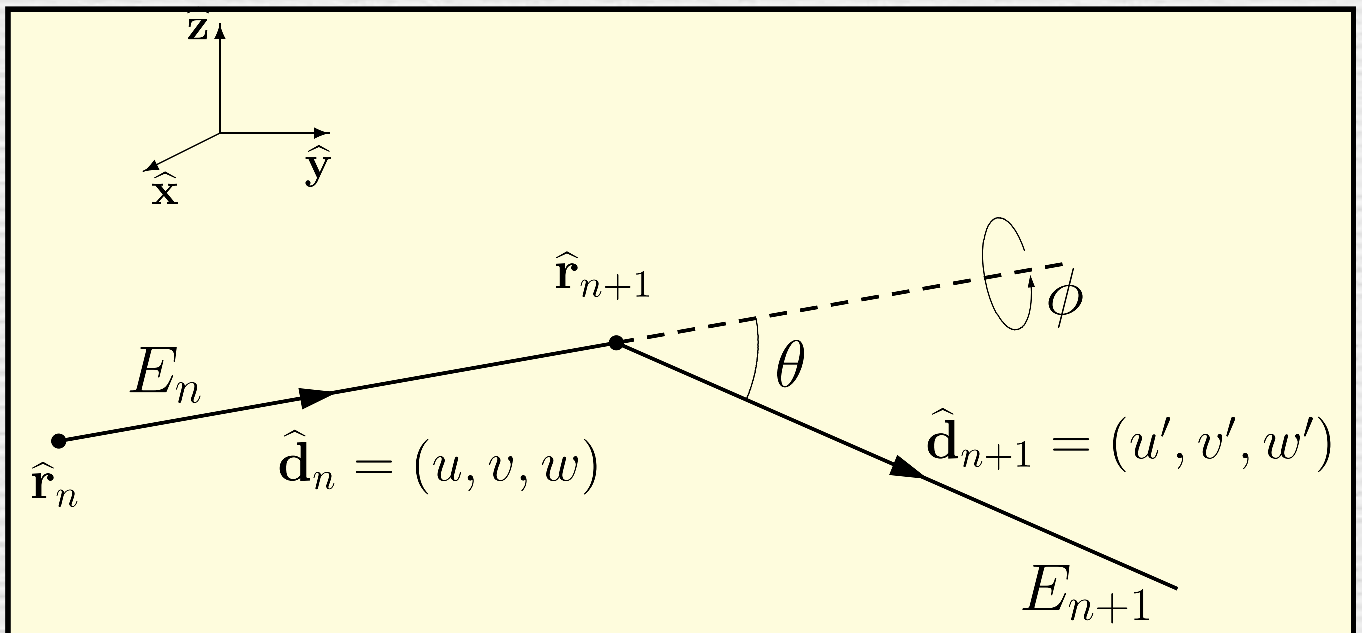
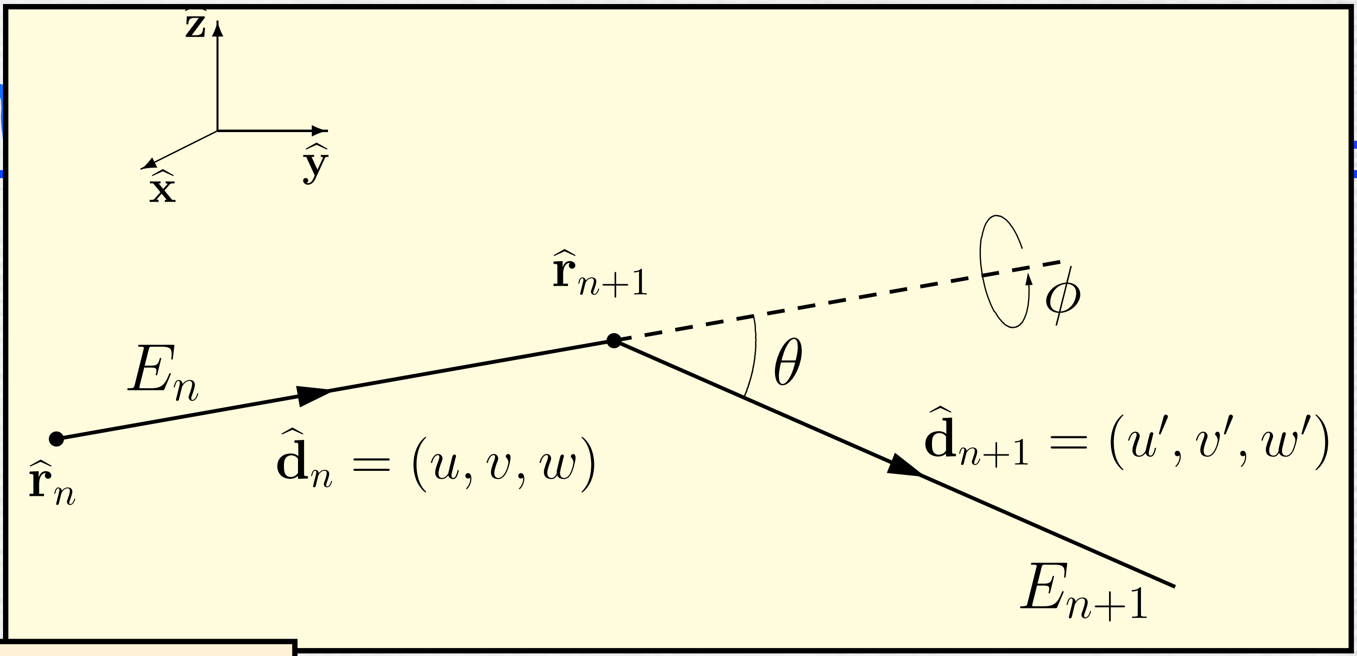


MC simulation of radiation



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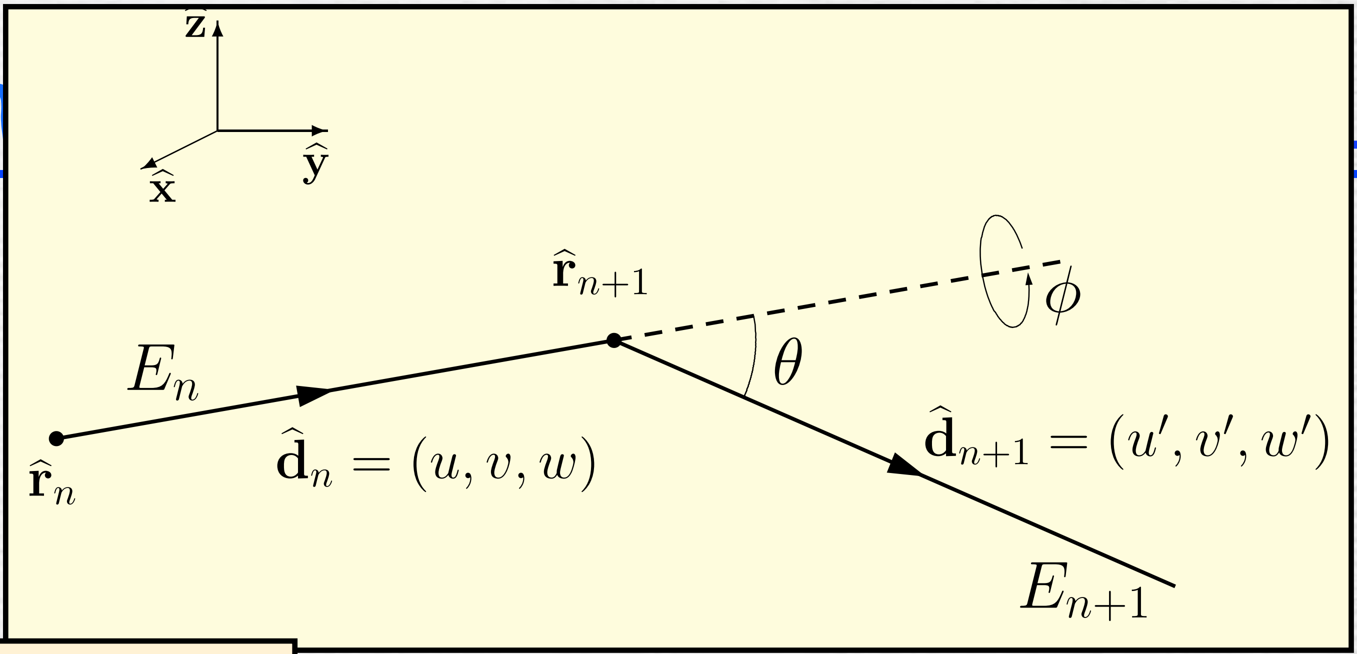

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¿A o B?

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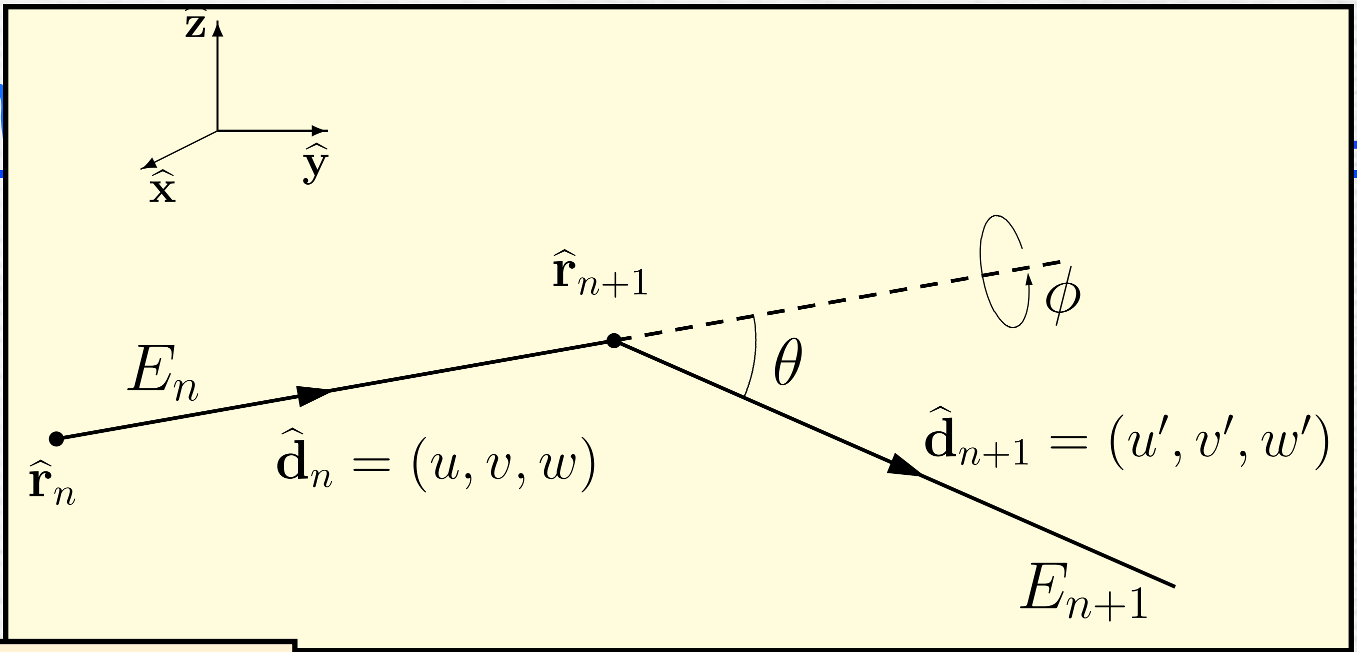

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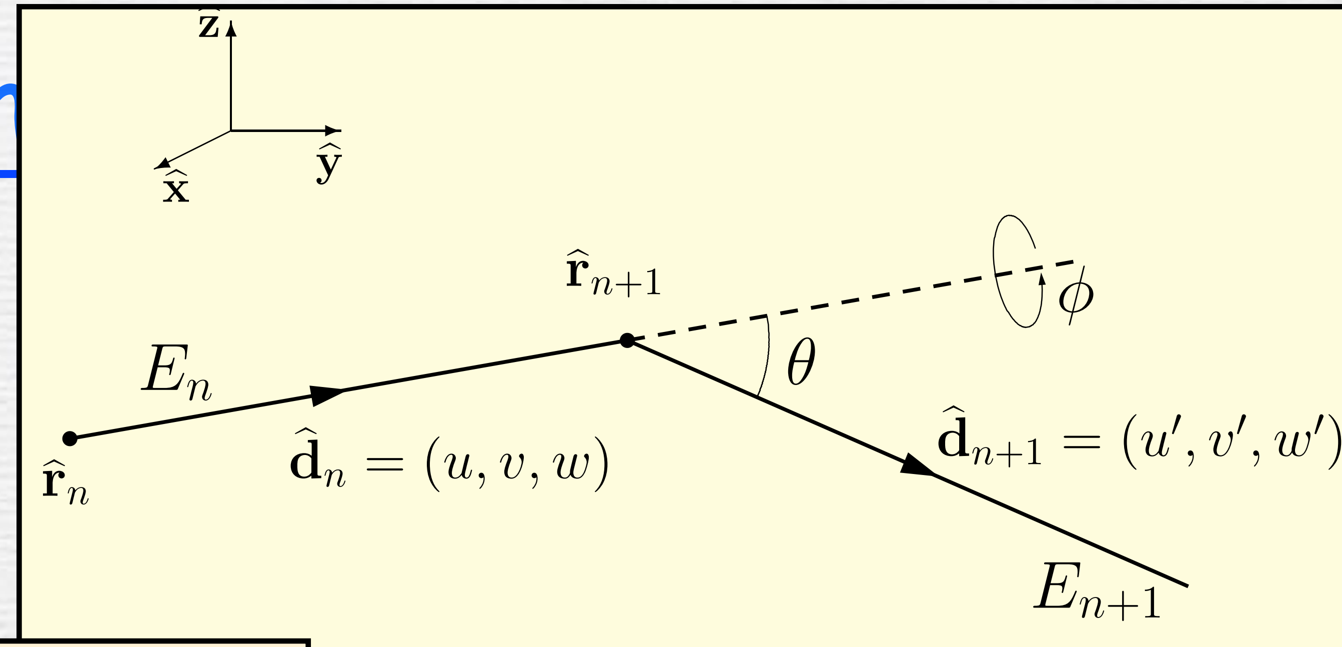

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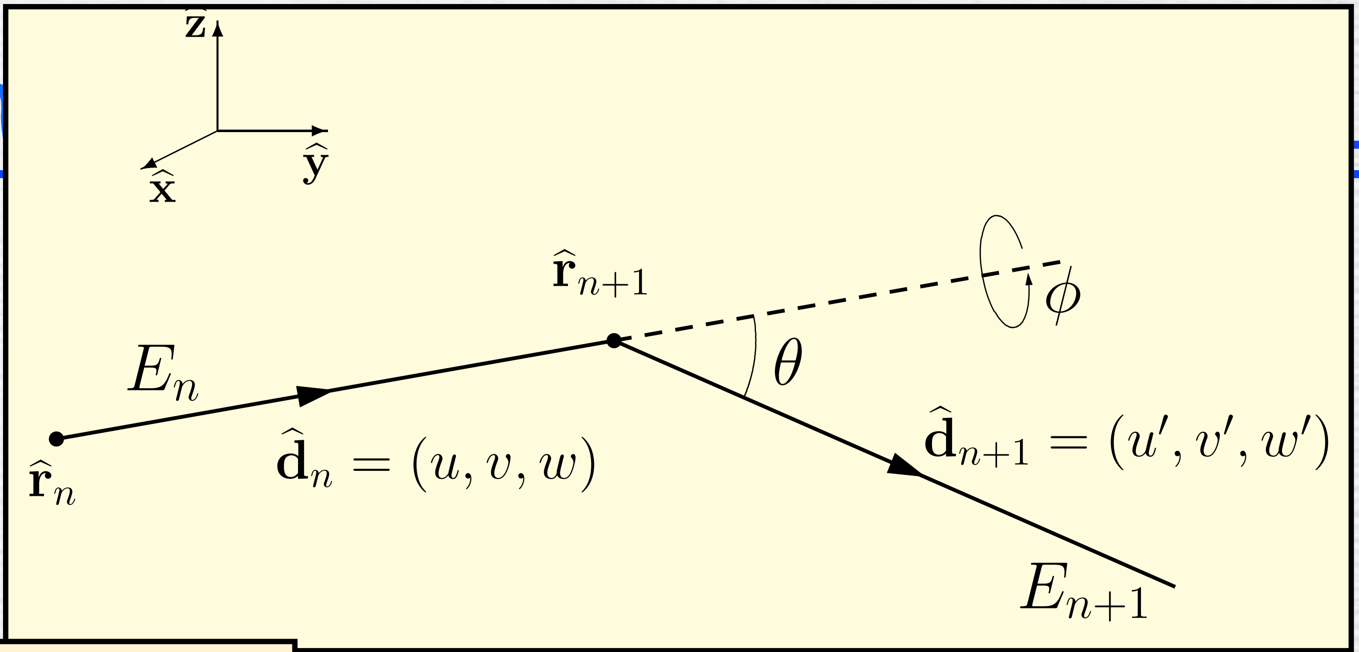

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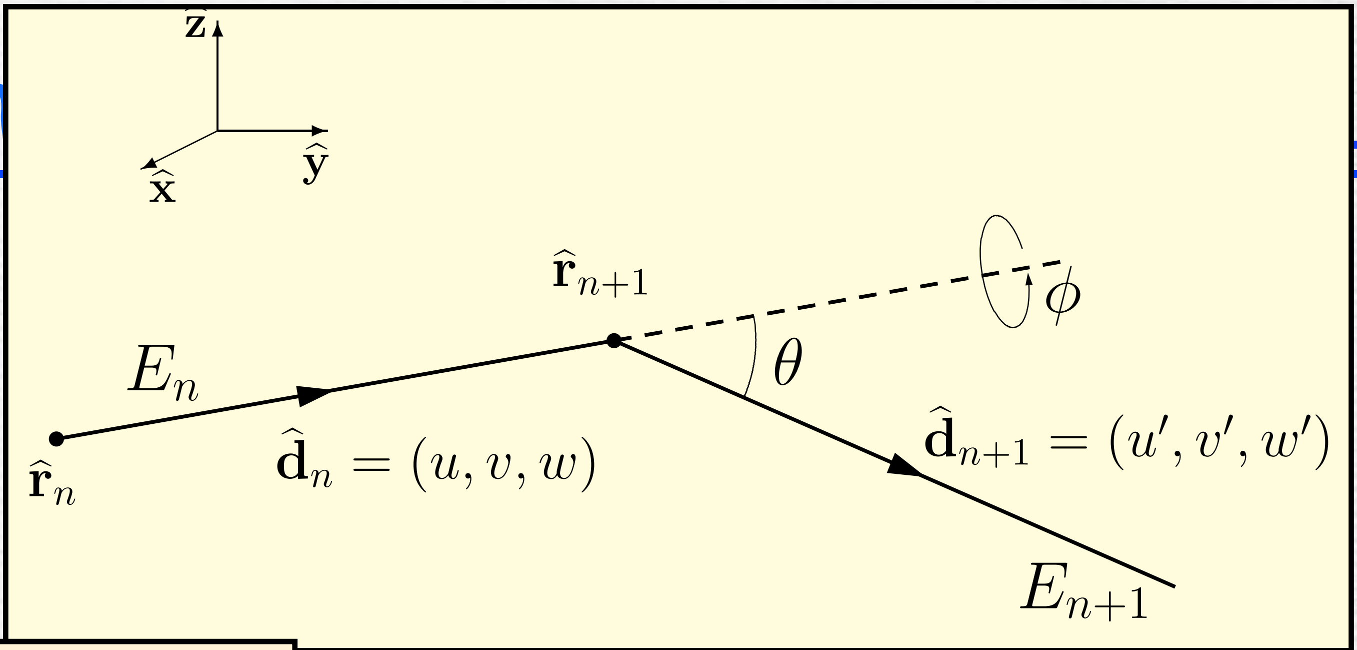

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$$E_{n+1} = E_n - W$$

$$\widehat{\mathbf{d}}_{n+1} = \mathcal{R}(\theta, \phi)\,\widehat{\mathbf{d}}_n$$

-determine W, θ and ϕ

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  - particle energy smaller than absorption energy
  - particle out of the material medium

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  - charged particles, other energies, etc.
  - how to sample probability distributions?

Random number generation

Uniform distibution U(0,1)

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- random numbers can be obtained in:

physical processes of random character

(radioactive processes, electric noise, etc.)

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$n_i \equiv$ number of disintegrations in Δt

$d_i \equiv 0$ or 1 according n_i being even or odd

$$
\begin{array}{cccccc}
i & 1 & 2 & 3 & & m \\
n_i & n_1 & n_2 & n_3 & \ldots & n_m \\
 & \downarrow & \downarrow & \downarrow & & \downarrow \\
d_i & 1 & 0 & 1 & \ldots & 1
\end{array}
$$

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VERY SLOW PROCESSES

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VERY SLOW PROCESSES ⟵

- tables

(p.ej.: Abramowitz and Stegun)

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  VERY SLOW PROCESSES ⟵

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same results are obtained than using

pseudo-ramdom numbers

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- algorithms based on congruence relations

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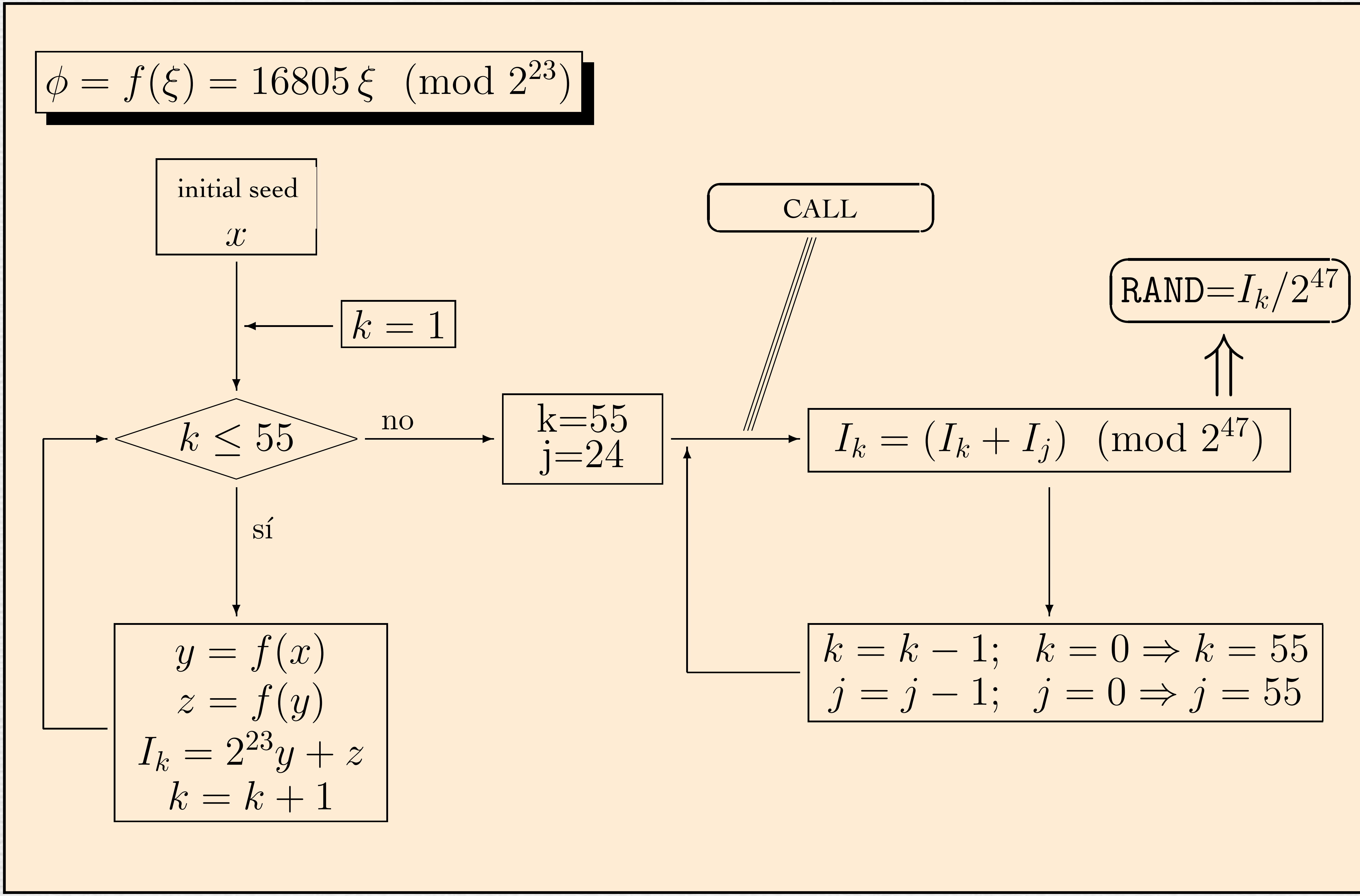
- basic rules:

  generated numbers: uncorrelated

  sequence: as long as possible

  generating algorithm: as quick as possible

Carlsson algorithm



Press W H, Teukolsky S A, Vetterling W T and Flannery B P
Numerical Recipes in Fortran 2nd ed.
New York: Cambridge University Press, 1992

```
      FUNCTION RAN1(IDUM)
      INTEGER IDUM,IA,IM,IQ,IR,NTAB,NDIV
      REAL RAN1,AM,EPS,RNMX
      PARAMETER (IA=16807,IM=2147483647,AM=1./IM,IQ=127773,IR=2836,
     >           NTAB=32,NDIV=1+(IM-1)/NTAB,EPS=1.2E-7,RNMX=1.-EPS)
      INTEGER J,K,IV(NTAB),IY
      SAVE IV,IY
      DATA IV /NTAB*0/, IY /0/
      IF (IDUM.LE.0.OR.IY.EQ.0) THEN
        IDUM=MAX(-IDUM,1)
        DO J=NTAB+8,1,-1
          K=IDUM/IQ
          IDUM=IA*(IDUM-K*IQ)-IR*K
          IF (IDUM.LT.0) IDUM=IDUM+IM
          IF (J.LE.NTAB) IV(J)=IDUM
        CONTINUE
        IY=IV(1)
      ENDIF
      K=IDUM/IQ
      IDUM=IA*(IDUM-K*IQ)-IR*K
      IF (IDUM.LT.0) IDUM=IDUM+IM
      J=1+IY/NDIV
      IY=IV(J)
      IV(J)=IDUM
      RAN1=MIN(AM*IY,RNMX)
      RETURN
      END
```

Random number generation

Other distributions

Random number generation

Other distributions

- inverse transform method
  (or variable change method)

- acceptance/rejection method

- Metropolis method
  (or random walk method)

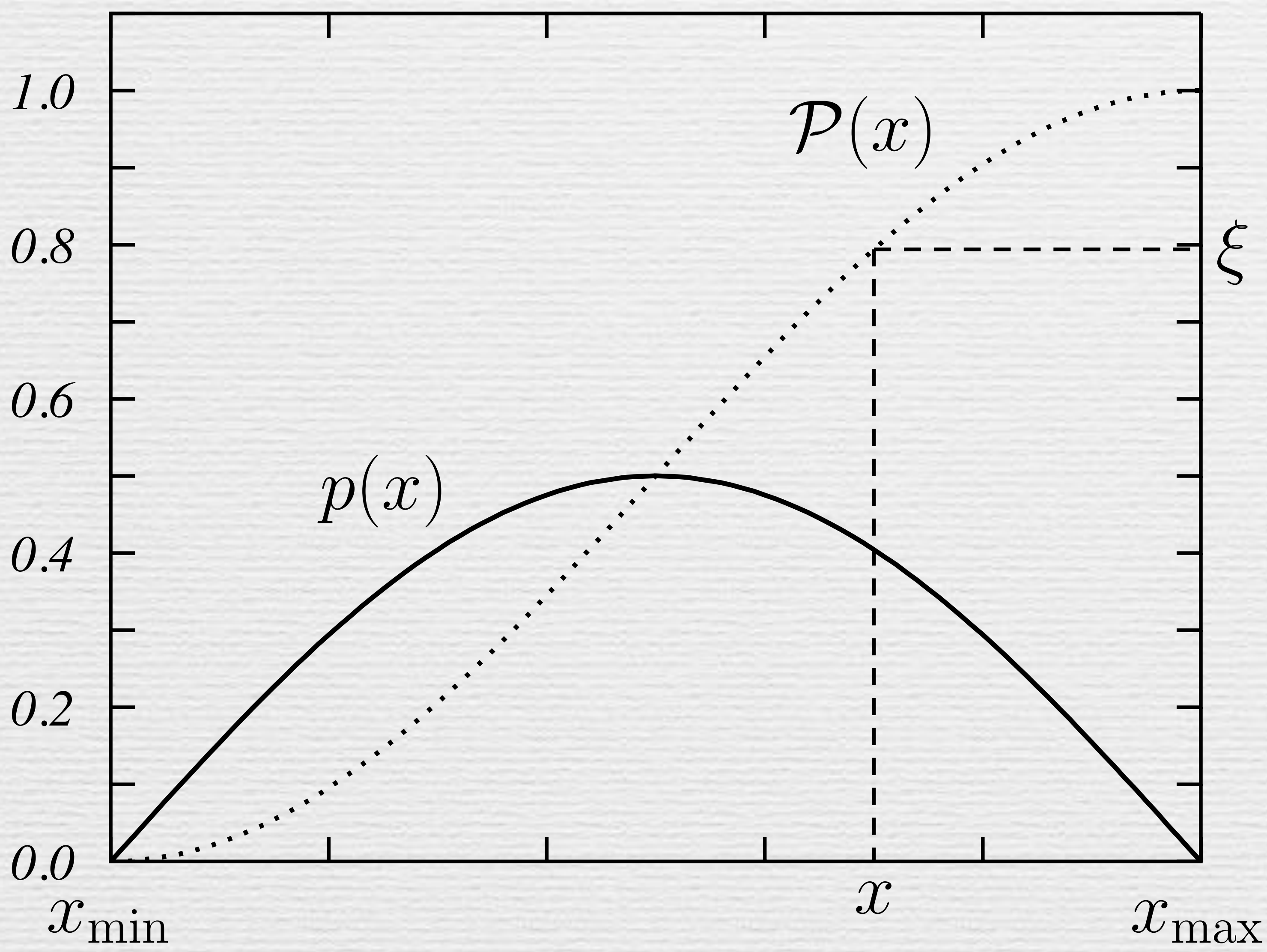
Random number generation

Other distributions: inverse transform method

Random number generation

Other distributions: inverse transform method

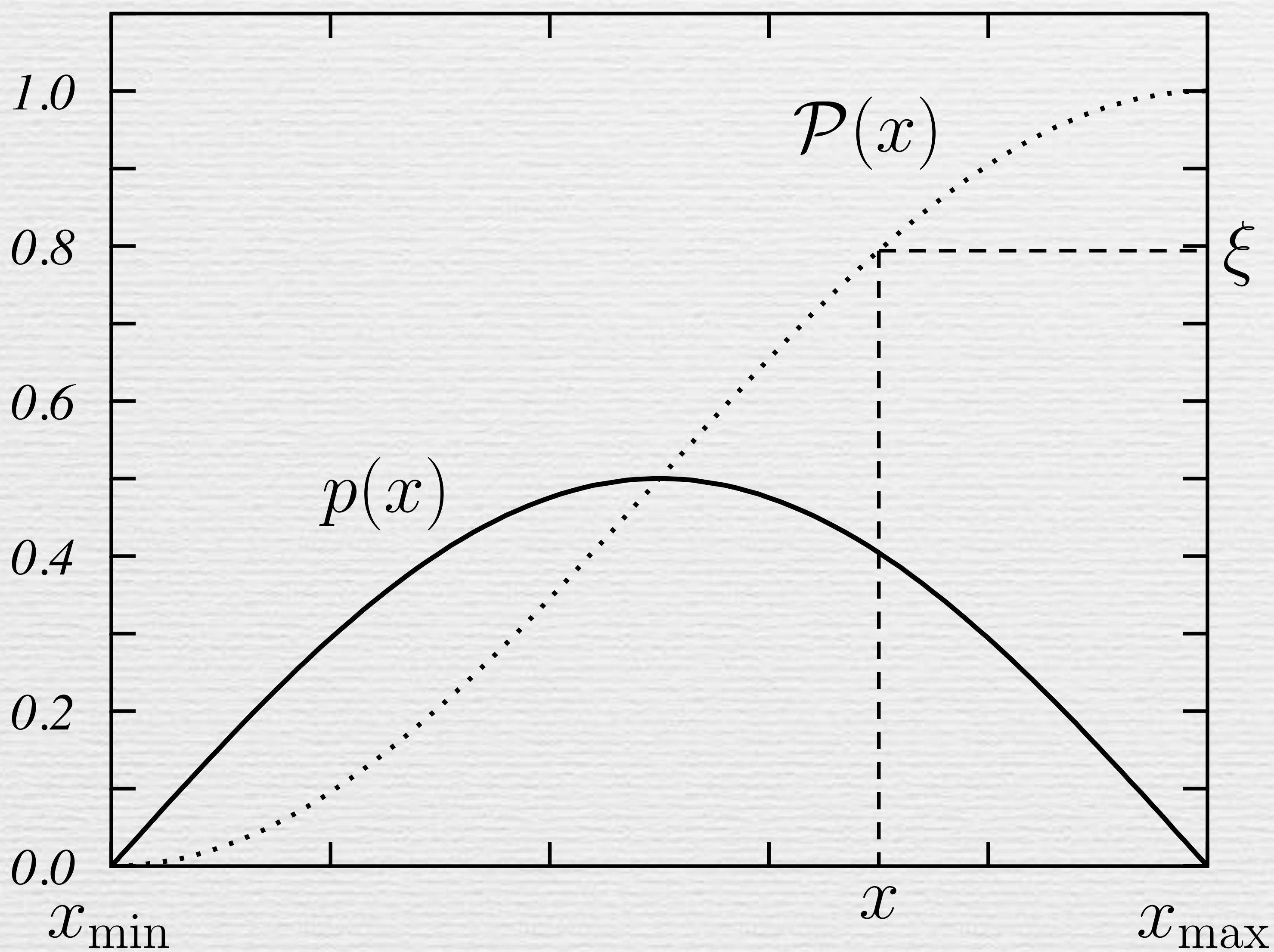
- to sample $\boxed{p(x),\ x \in (x_{\min}, x_{\max})}$



Random number generation

Other distributions: inverse transform method

- to sample $p(x),\ x \in (x_{\min}, x_{\max})$

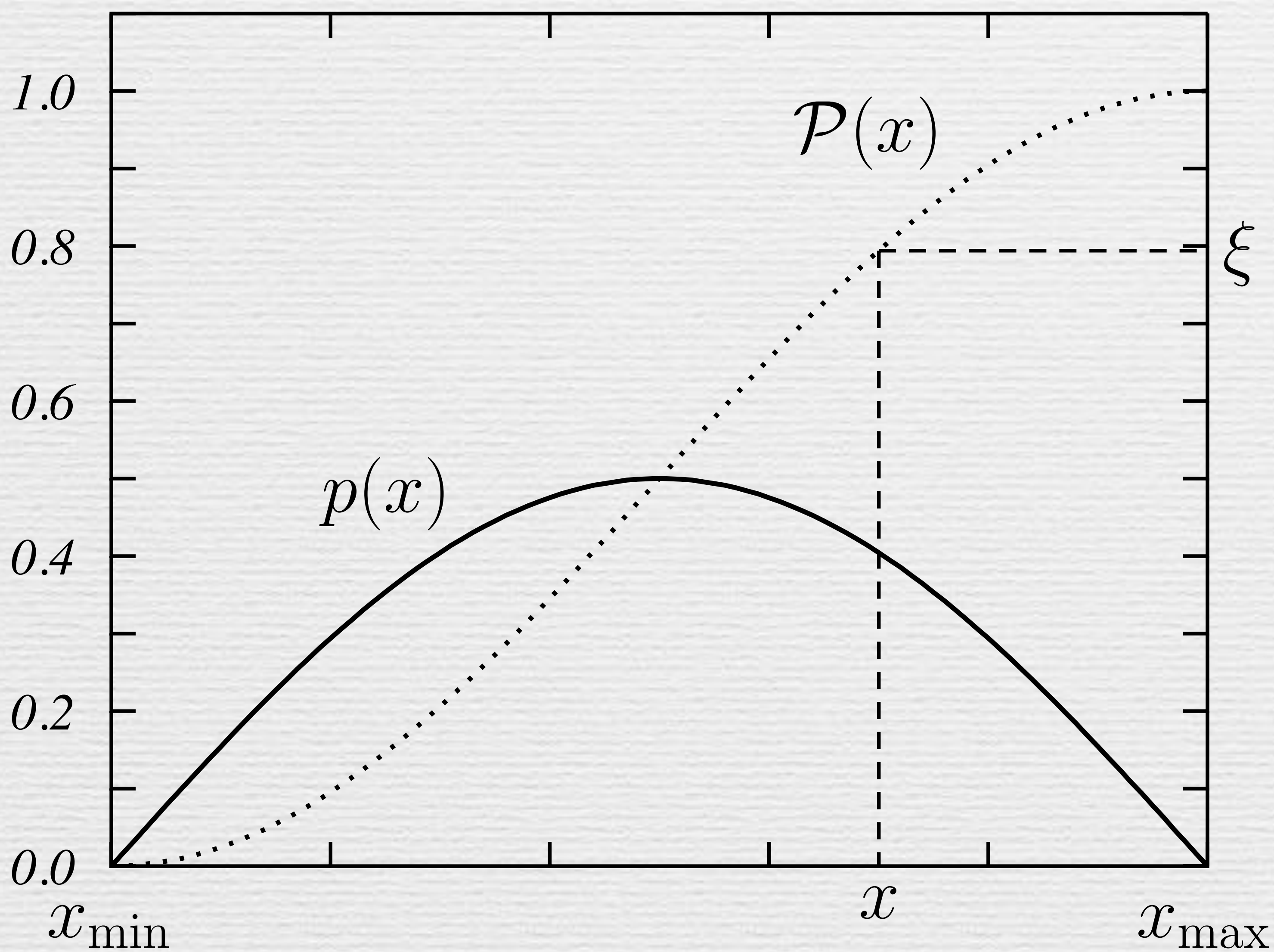


$$\mathcal{P}(x) \equiv \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

Random number generation

Other distributions: inverse transform method

- to sample $\boxed{p(x),\ x \in (x_{\min}, x_{\max})}$



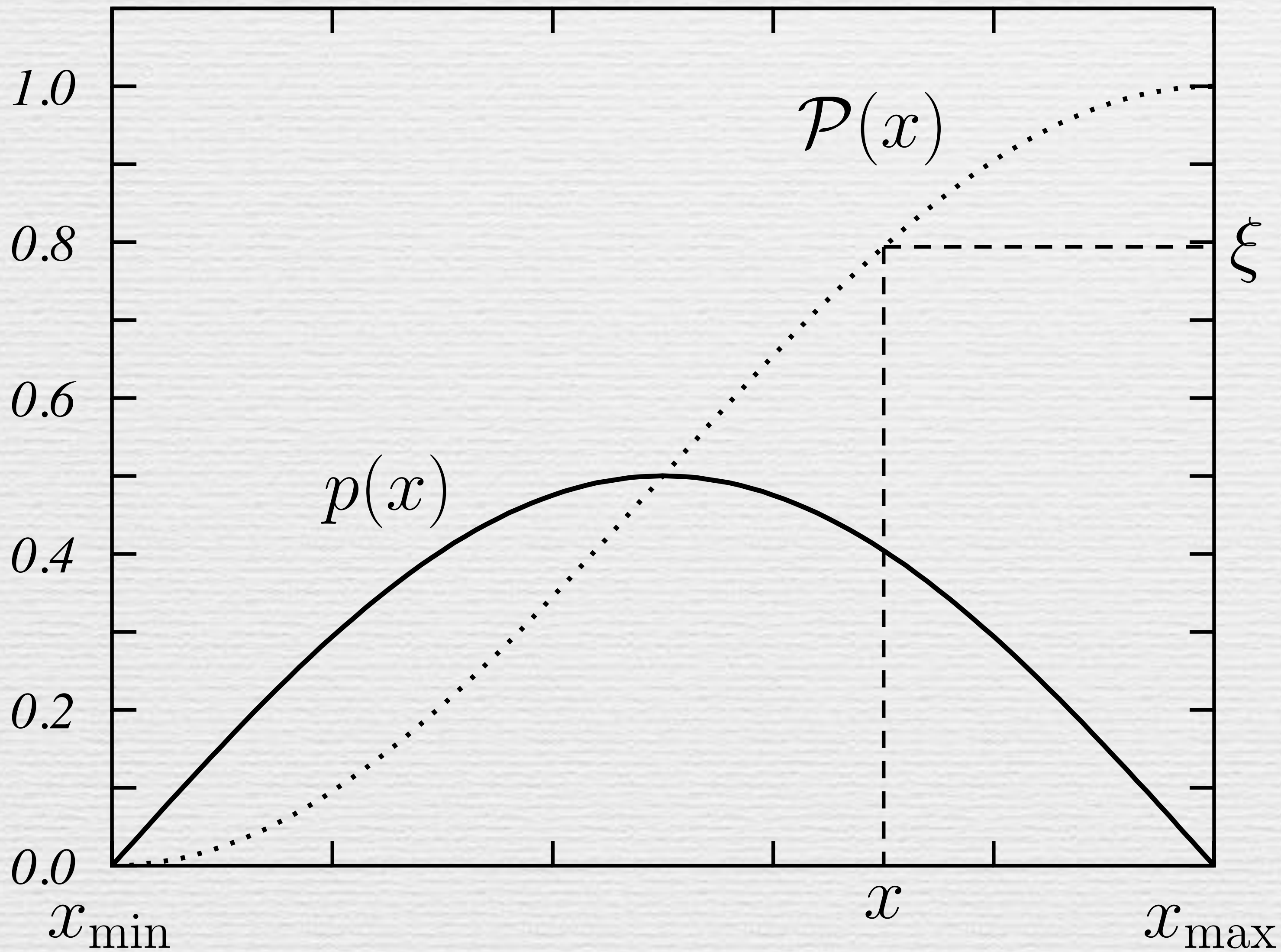
$$\boxed{\mathcal{P}(x) \equiv \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)}$$

$$\boxed{x = \mathcal{P}^{-1}(\xi)\,, \quad \xi \in U(0,1)}$$

Random number generation

Other distributions: inverse transform method

- to sample $p(x),\ x \in (x_{\min}, x_{\max})$



$$\mathcal{P}(x) \equiv \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

$$x = \mathcal{P}^{-1}(\xi)\,,\quad \xi \in U(0,1)$$

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

- to sample: uniform PDF

$$p(x) \equiv U(a,b) = \frac{1}{b-a}, \quad \forall x \in (a,b)$$

Random number generation

Other distributions: inverse transform method

- to sample: uniform PDF

$$p(x) \equiv U(a,b) = \frac{1}{b-a}, \quad \forall x \in (a,b)$$

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

$$\xi = \int_{a}^{x} \mathrm{d}y\, \frac{1}{b-a} = \frac{x-a}{b-a}$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

- to sample: uniform PDF

$$p(x) \equiv U(a,b) = \frac{1}{b-a}\,, \quad \forall x \in (a,b)$$

$$\xi = \int_a^x \mathrm{d}y\, \frac{1}{b-a} = \frac{x-a}{b-a}$$

$$x = a + (b-a)\,\xi\,, \quad \xi \in U(0,1)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

Random number generation

Other distributions: inverse transform method

- to sample: exponential PDF

$$p(x) = \frac{1}{\lambda} \exp\left(-\frac{x}{\lambda}\right) , \quad x > 0$$

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

Random number generation

Other distributions: inverse transform method

- to sample: exponential PDF

$$p(x) = \frac{1}{\lambda} \exp\left(-\frac{x}{\lambda}\right) \ , \quad x > 0$$

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

$$\xi = \int_0^x \mathrm{d}y \left[\frac{1}{\lambda} \exp\left(-\frac{y}{\lambda}\right)\right] = 1 - \exp\left(-\frac{x}{\lambda}\right)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

- to sample: exponential PDF

$$p(x) = \frac{1}{\lambda} \exp\left(-\frac{x}{\lambda}\right) , \quad x > 0$$

$$\xi = \int_0^x \mathrm{d}y \left[\frac{1}{\lambda} \exp\left(-\frac{y}{\lambda}\right)\right] = 1 - \exp\left(-\frac{x}{\lambda}\right)$$

$$x = -\lambda \ln(1 - \xi) , \quad \xi \in U(0,1)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

- to sample: exponential PDF

$$p(x) = \frac{1}{\lambda} \exp\left(-\frac{x}{\lambda}\right) , \quad x > 0$$

$$\xi = \int_0^x \mathrm{d}y \left[\frac{1}{\lambda} \exp\left(-\frac{y}{\lambda}\right)\right] = 1 - \exp\left(-\frac{x}{\lambda}\right)$$

$$x = -\lambda \ln(1-\xi) , \quad \xi \in U(0,1)$$

$$x = -\lambda \ln \xi , \quad \xi \in U(0,1)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

Random number generation

Other distributions: inverse transform method

- to sample: Gaussian PDF

$$p_{\mathrm{G}}(x) = N(0,1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y \, p(y)$$

- to sample: Gaussian PDF

$$p_{\mathrm{G}}(x) = N(0,1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

$$p(x_1, x_2) = p_{\mathrm{G}}(x_1)\, p_{\mathrm{G}}(x_2) = \frac{1}{2\pi} \exp\left(-\frac{x_1^2 + x_2^2}{2}\right)$$

$$p(x_1, x_2)\, \mathrm{d}x_1\, \mathrm{d}x_2 = \left[r \exp\left(-\frac{r^2}{2}\right) \mathrm{d}r \right] \left[\frac{1}{2\pi} \mathrm{d}\phi \right]$$

Random number generation

Other distributions: inverse transform method

sampling equation

$$\xi = \int_{x_{\min}}^{x} \mathrm{d}y\, p(y)$$

- to sample: Gaussian PDF

$$p_{\mathrm{G}}(x) = N(0,1) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

$$p(x_1,x_2) = p_{\mathrm{G}}(x_1)\, p_{\mathrm{G}}(x_2) = \frac{1}{2\pi} \exp\left(-\frac{x_1^2+x_2^2}{2}\right)$$

$$p(x_1,x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 = \left[r \exp\left(-\frac{r^2}{2}\right) \mathrm{d}r\right] \left[\frac{1}{2\pi}\mathrm{d}\phi\right]$$

$$\begin{aligned} x_1 &= \sqrt{-2\ln\xi_1}\, \cos(2\pi\xi_2) \\ x_2 &= \sqrt{-2\ln\xi_1}\, \sin(2\pi\xi_2) \end{aligned} \quad , \quad \xi_1,\xi_2 \in U(0,1)$$

Box-Müller method

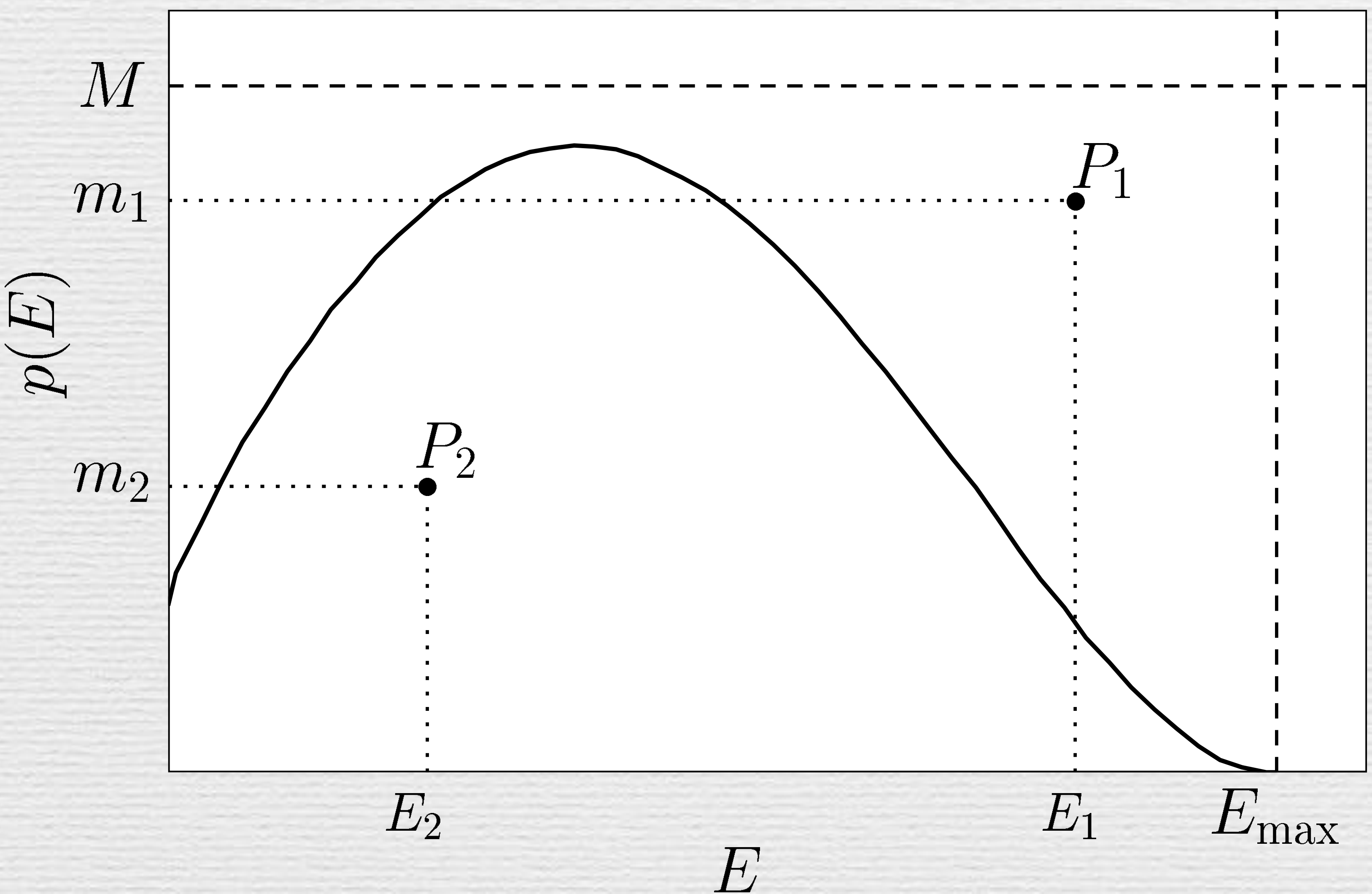
Random number generation

Other distributions: acceptance/rejection method

Random number generation

Other distributions: acceptance/rejection method

- to sample $\boxed{p(E)\,, E \in (0, E_{\max})}$

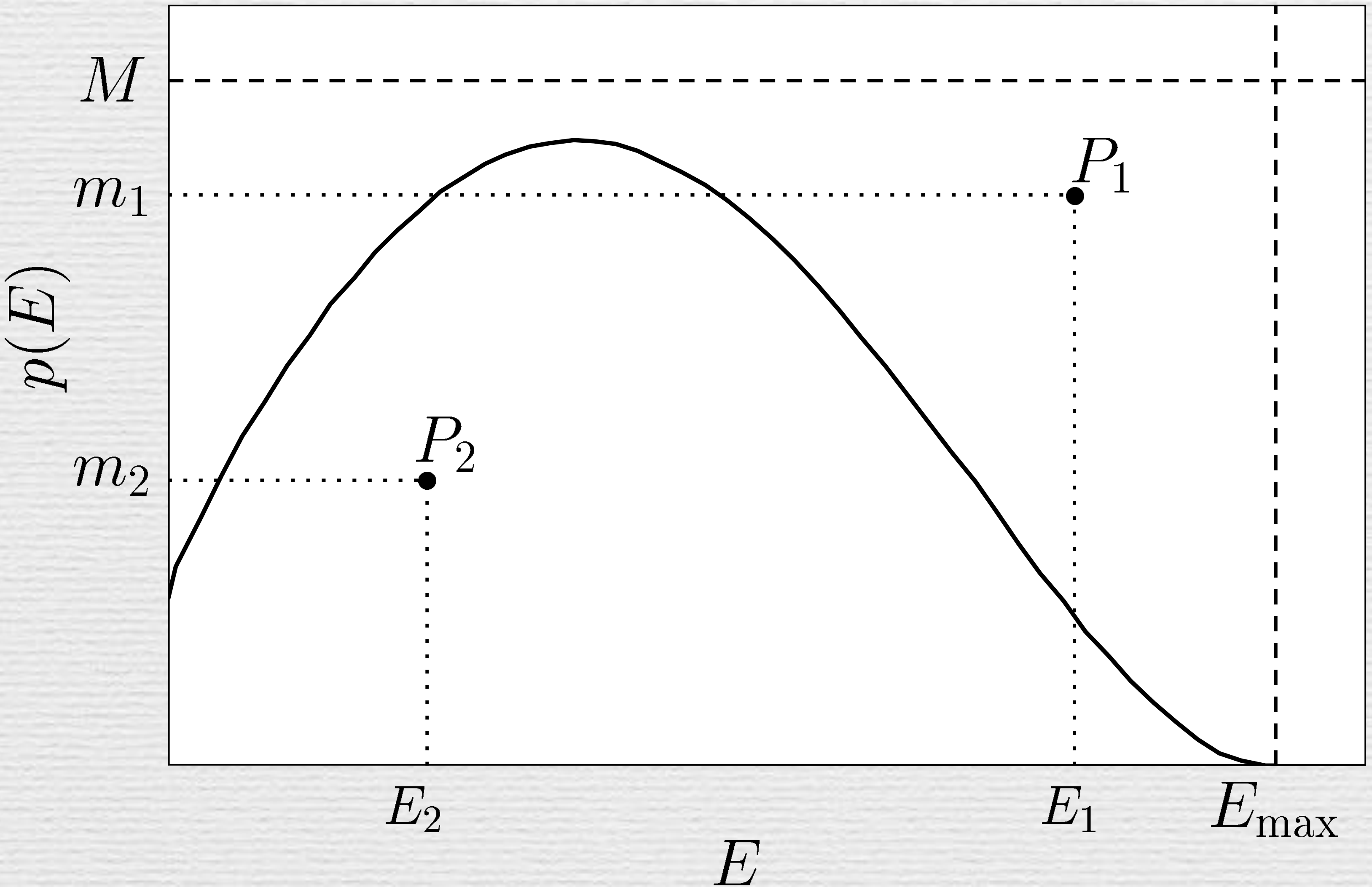


Random number generation

Other distributions: acceptance/rejection method

- to sample $\boxed{p(E)\,,\, E \in (0, E_{\max})}$

-let us define $\boxed{M \mid p(E) \,<\, M\,,\;\; \forall\, E \,\in\, [0, E_{\max}]}$



Random number generation

Other distributions: acceptance/rejection method

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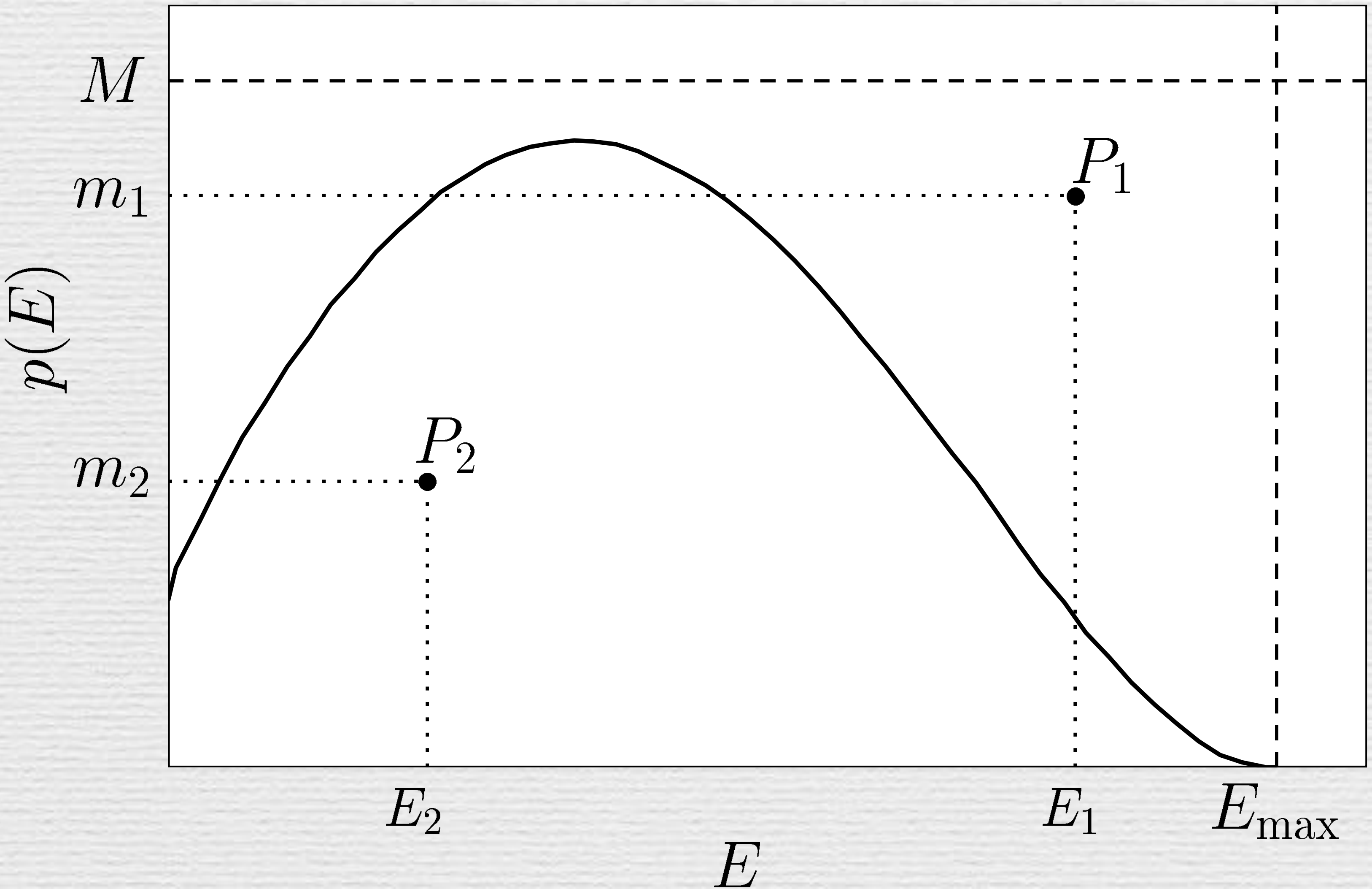
-let us define $\boxed{M \mid p(E) \,<\, M\,,\;\; \forall\, E \,\in\, [0, E_{\max}]}$

-we generate $\boxed{E_i \in U(0, E_{\max})\,,\; m_i \in U(0, M)}$



Random number generation

Other distributions: acceptance/rejection method

- to sample $\boxed{p(E)\,,\, E \in (0, E_{\max})}$

-let us define $\boxed{M \mid p(E) < M\,,\ \forall E \in [0, E_{\max}]}$

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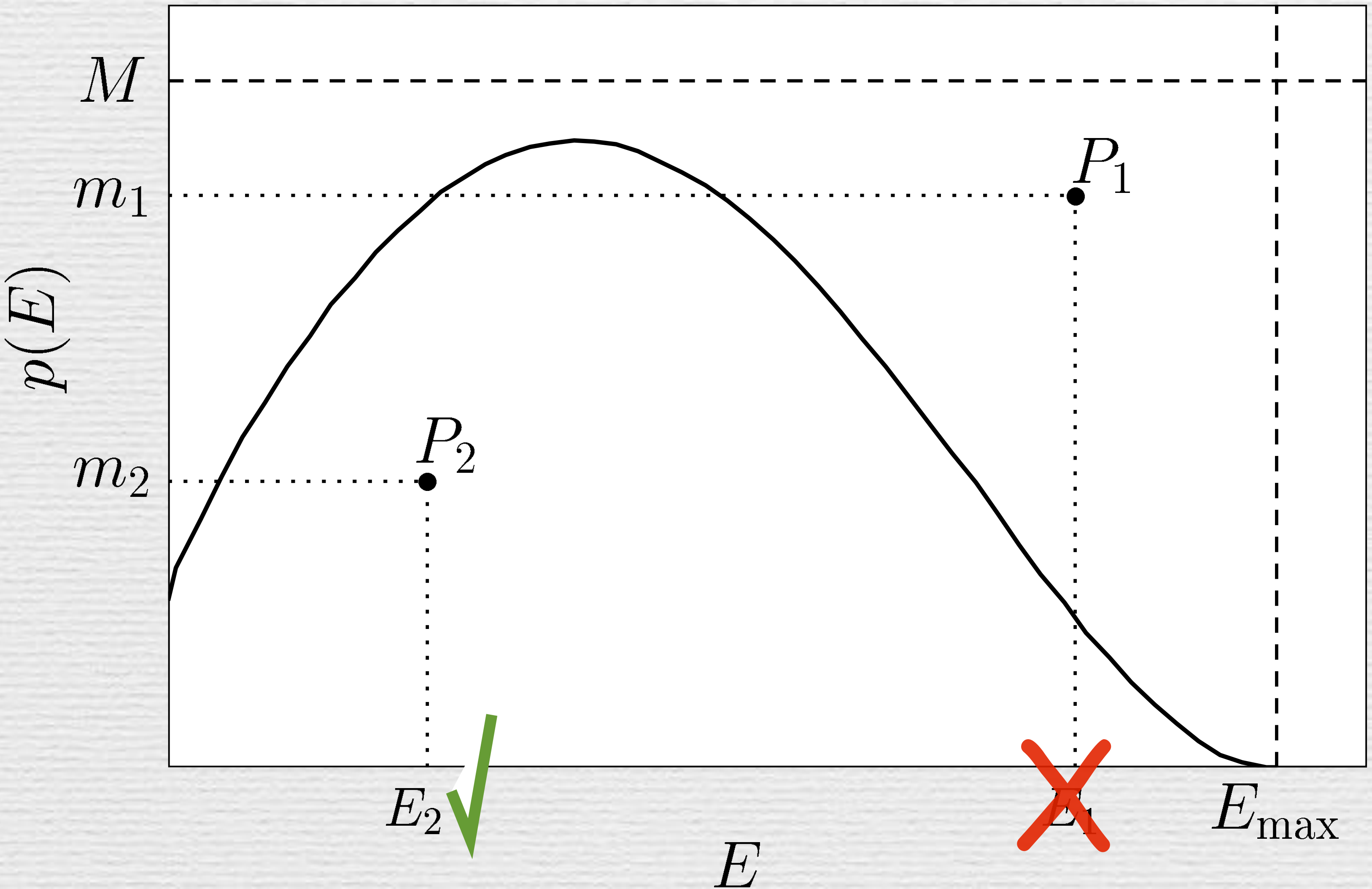


if $p(E_i) \geq m_i$
E_i is accepted

Random number generation

Other distributions: Metropolis method

- to sample any $p(x)$

Other distributions: Metropolis method

- to sample any $p(x)$

(x_0, D)

Random number generation

Other distributions: Metropolis method

- to sample any $p(x)$

$$\boxed{(x_0, D)} \rightarrow \boxed{\xi \in U(0,1)}$$

Random number generation

Other distributions: Metropolis method

- to sample any $p(x)$

(x_0, D) → $\xi \in U(0,1)$ → $x_i = x_{i-1} + D(2\,\xi - 1)$

Random number generation

Other distributions: Metropolis method

- to sample any $p(x)$

$$(x_0, D) \rightarrow \xi \in U(0,1) \rightarrow x_i = x_{i-1} + D(2\,\xi - 1)$$

$$\downarrow$$

$$p(x_i) \geq p(x_{i-1})$$

Random number generation

Other distributions: Metropolis method

- to sample any $p(x)$

(x_0, D) → $\xi \in U(0,1)$ → $x_i = x_{i-1} + D(2\,\xi - 1)$

$p(x_i) \geq p(x_{i-1})$

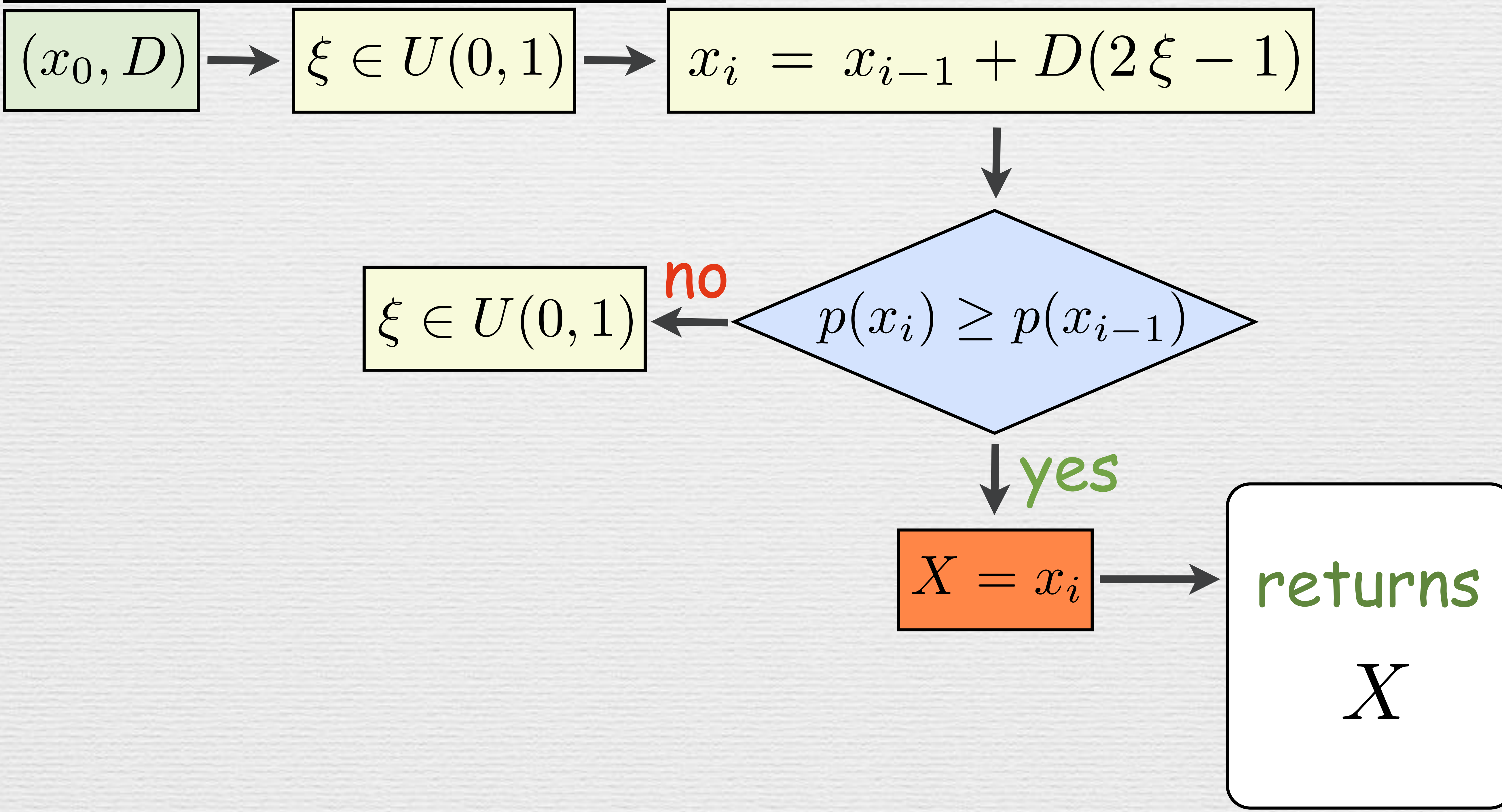
yes

$X = x_i$ → returns X

Random number generation

Other distributions: Metropolis method

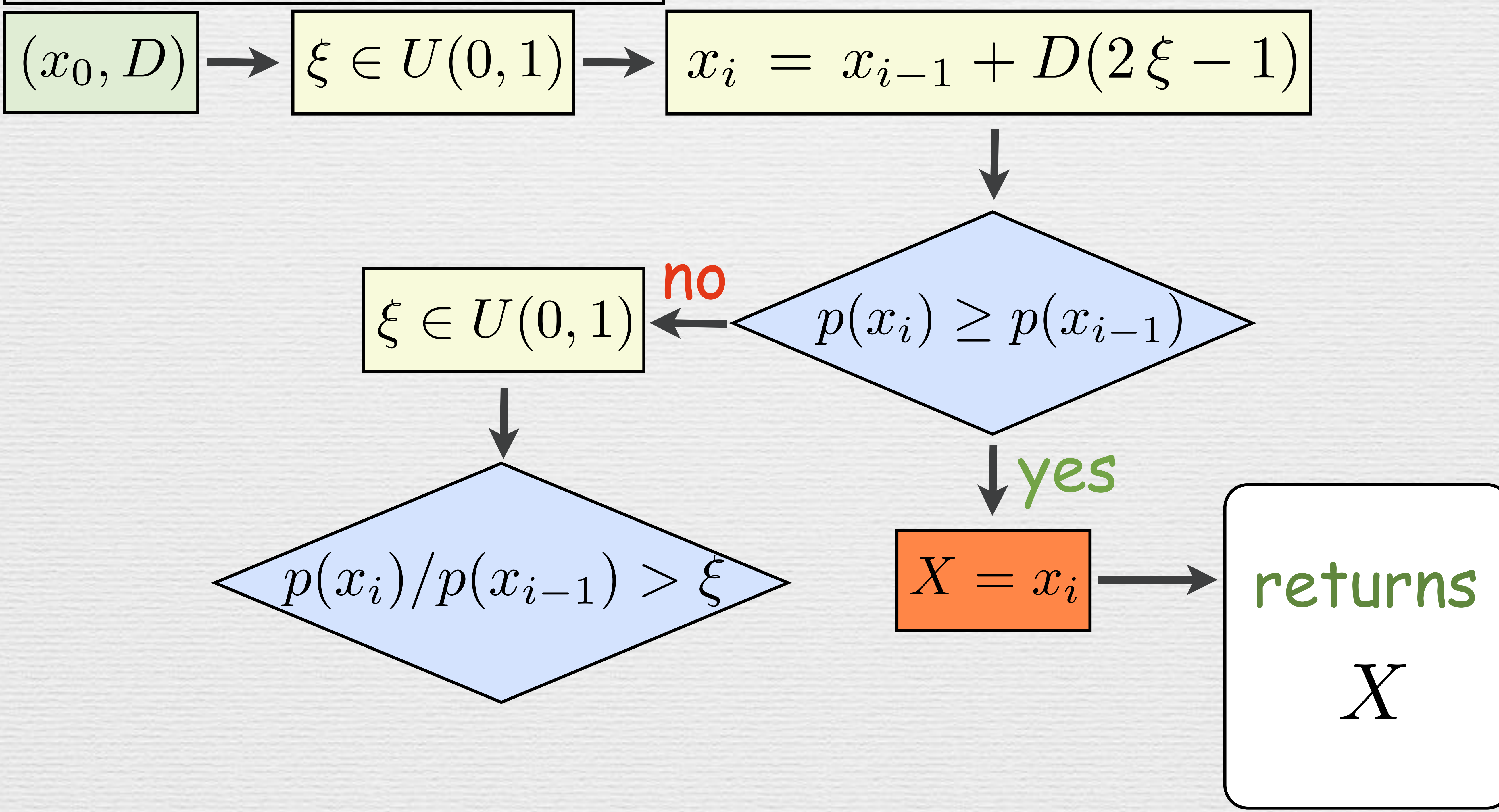
- to sample any $p(x)$



Random number generation

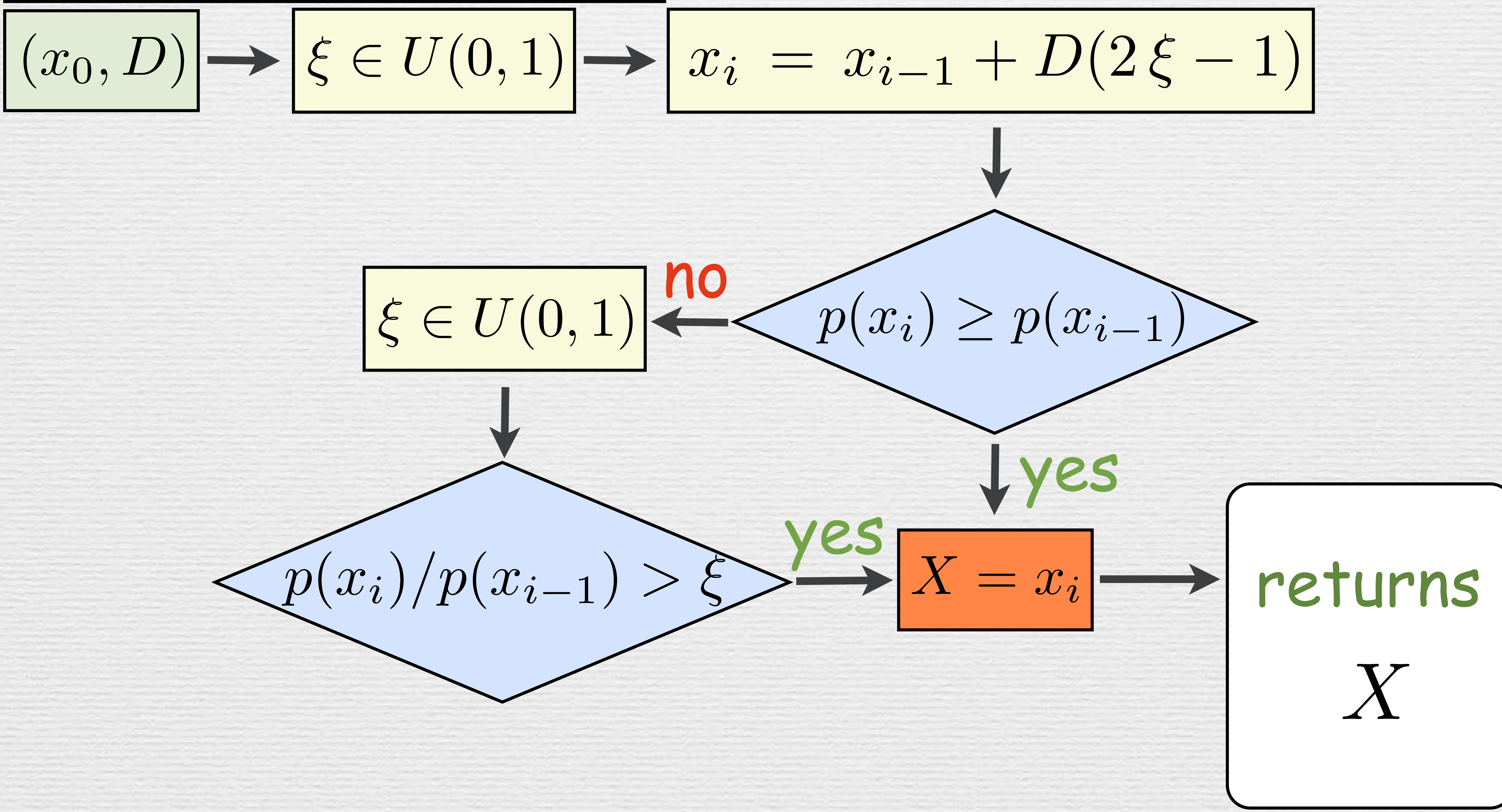
Other distributions: Metropolis method

- to sample any $p(x)$



Other distributions: Metropolis method

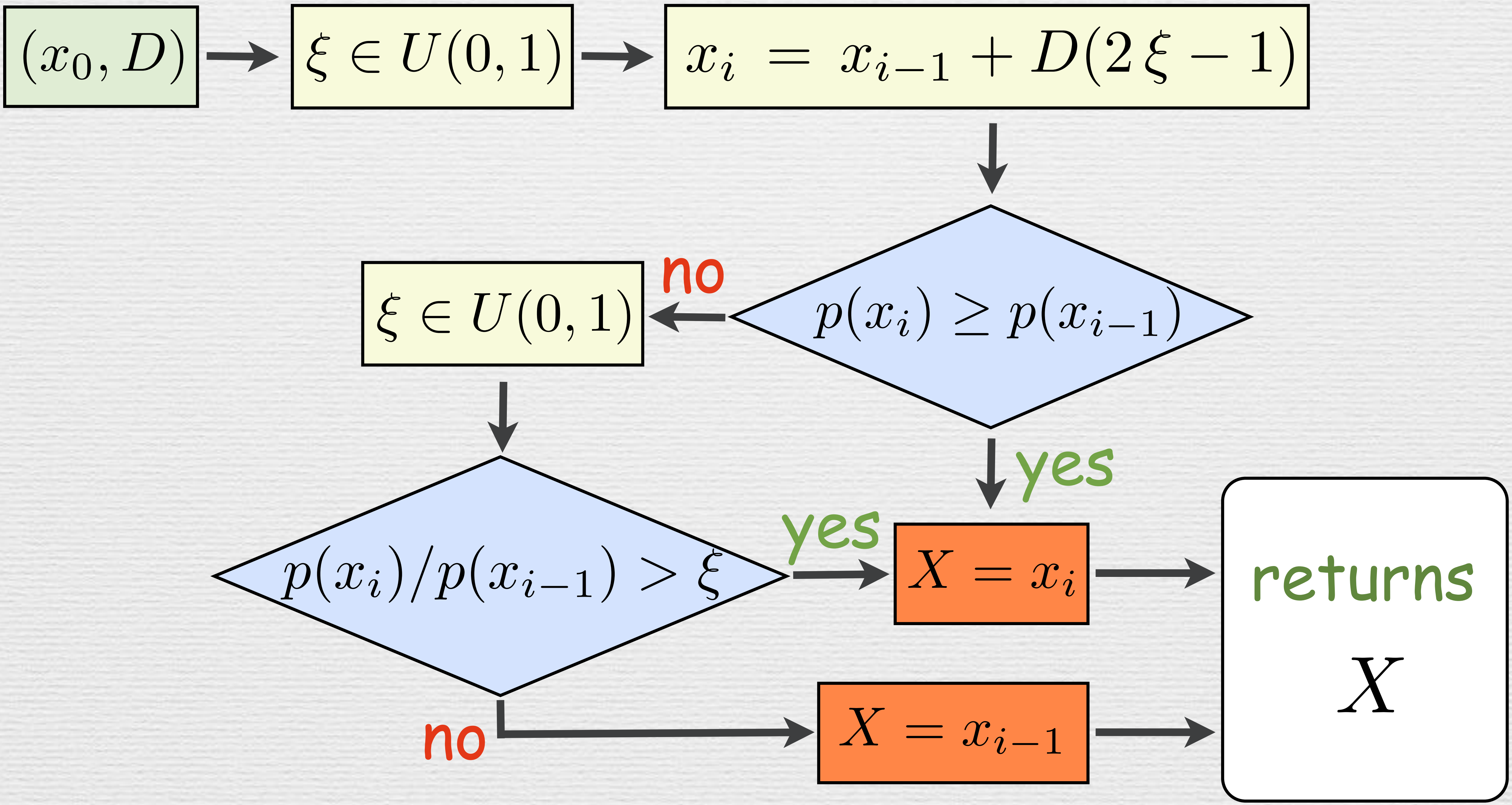
- to sample any $p(x)$



Random number generation

Other distributions: Metropolis method

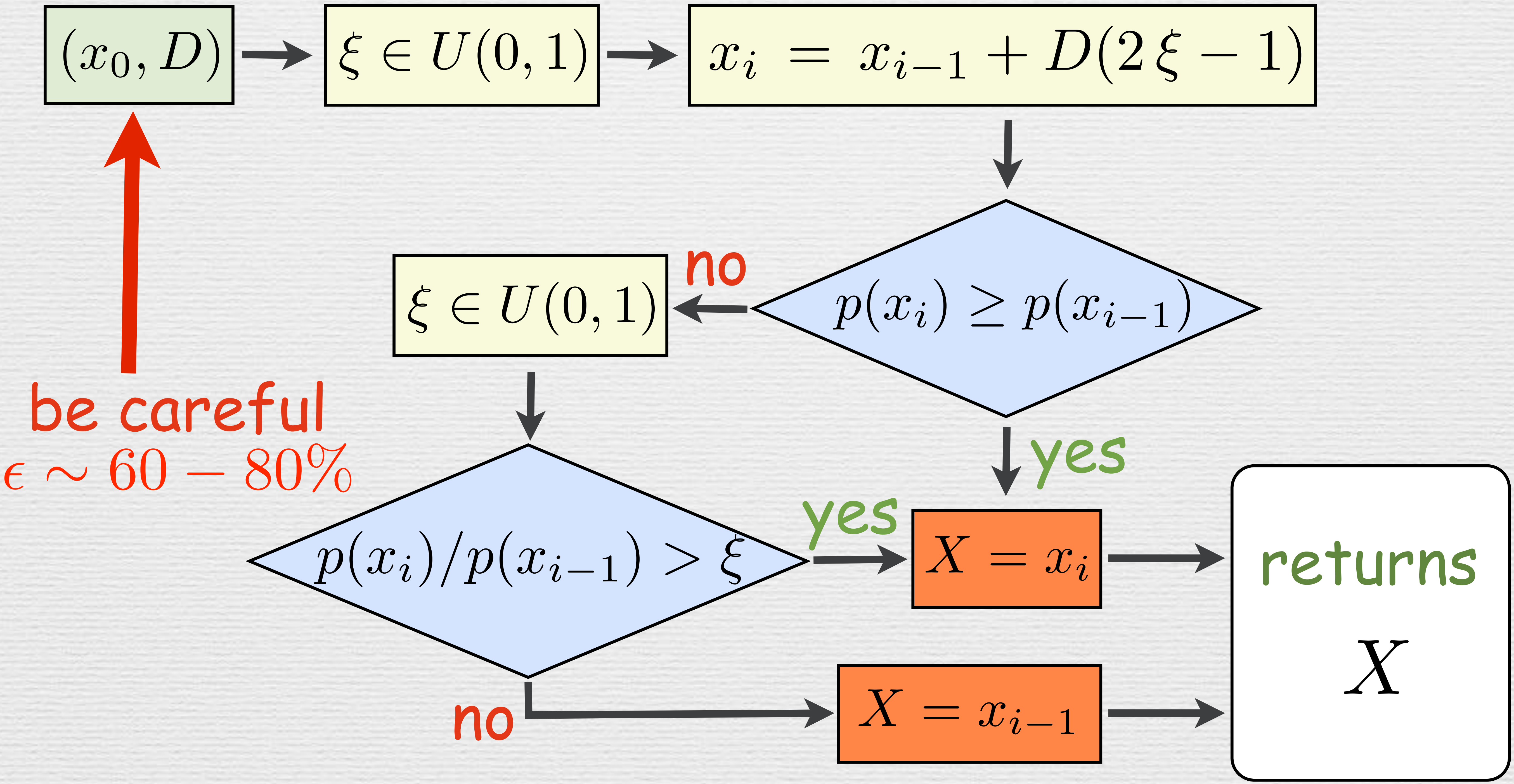
- to sample any $p(x)$



Random number generation

Other distributions: Metropolis method

- to sample any $p(x)$



Simple exercises

Sampling distributions

Simple exercises

Sampling distributions

1. choose a probability distribution

Simple exercises

Sampling distributions

1. choose a probability distribution
2. sample the distribution using the algorithms just described

Simple exercises

Sampling distributions

1. choose a probability distribution
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3. build up the histogram corresponding to the numbers obtained in the sampling

Simple exercises

Sampling distributions

1. choose a probability distribution
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CHANGE BIN SIZE AND NUMBER!!!

Simple exercises

Sampling distributions

1. choose a probability distribution
2. sample the distribution using the algorithms just described
3. build up the histogram corresponding to the numbers obtained in the sampling

   CHANGE BIN SIZE AND NUMBER!!!
4. compare distribution and histogram

Simple exercises

Sampling distributions

1. choose a probability distribution
2. sample the distribution using the algorithms just described
3. build up the histogram corresponding to the numbers obtained in the sampling

   CHANGE BIN SIZE AND NUMBER!!!
4. compare distribution and histogram

   NORMALIZATION!!!

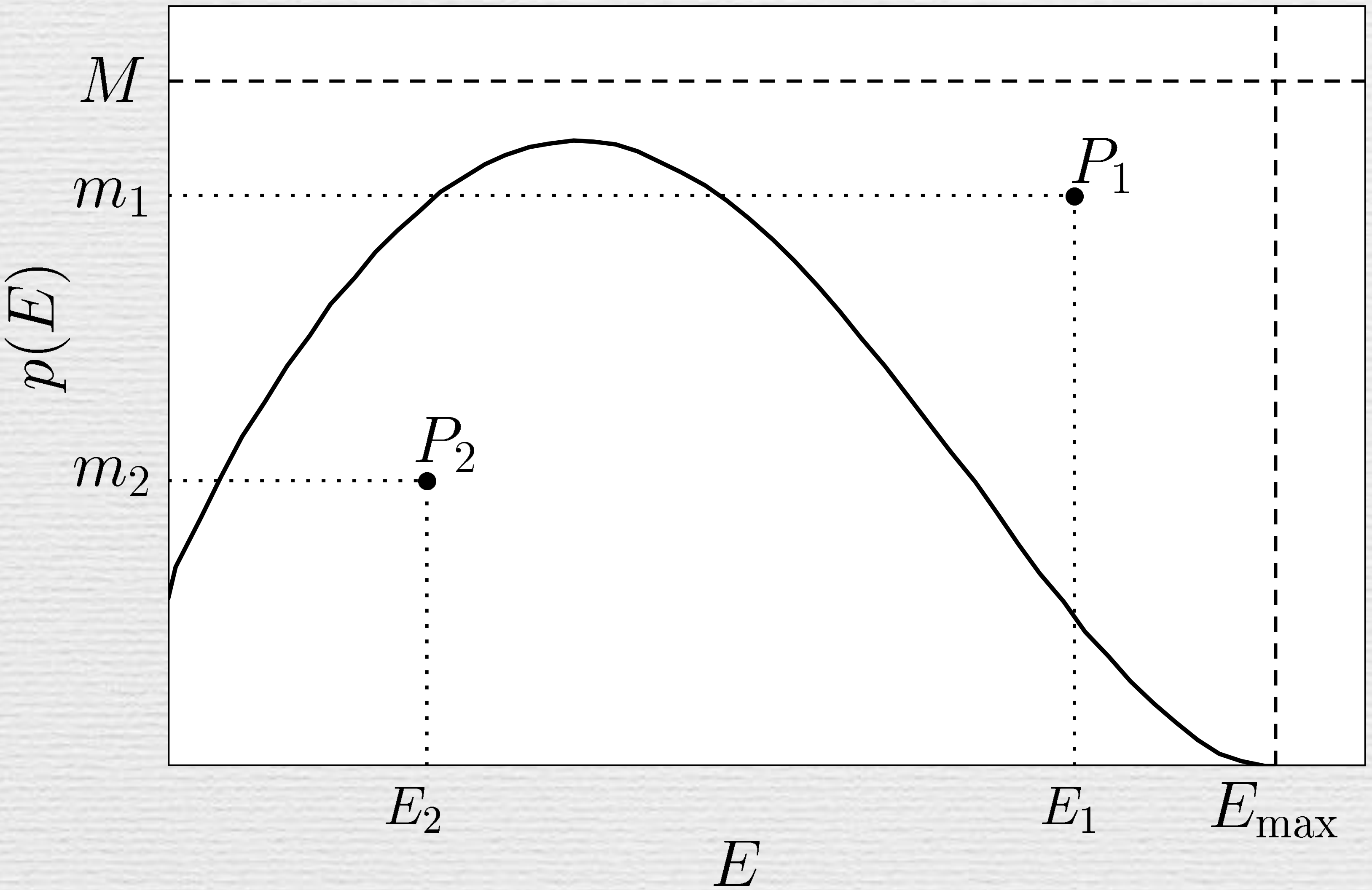
Simple exercises

Integral calculation

Simple exercises

Integral calculation

$$I = \int_0^{E_{\max}} \mathrm{d}E \, p(E)$$

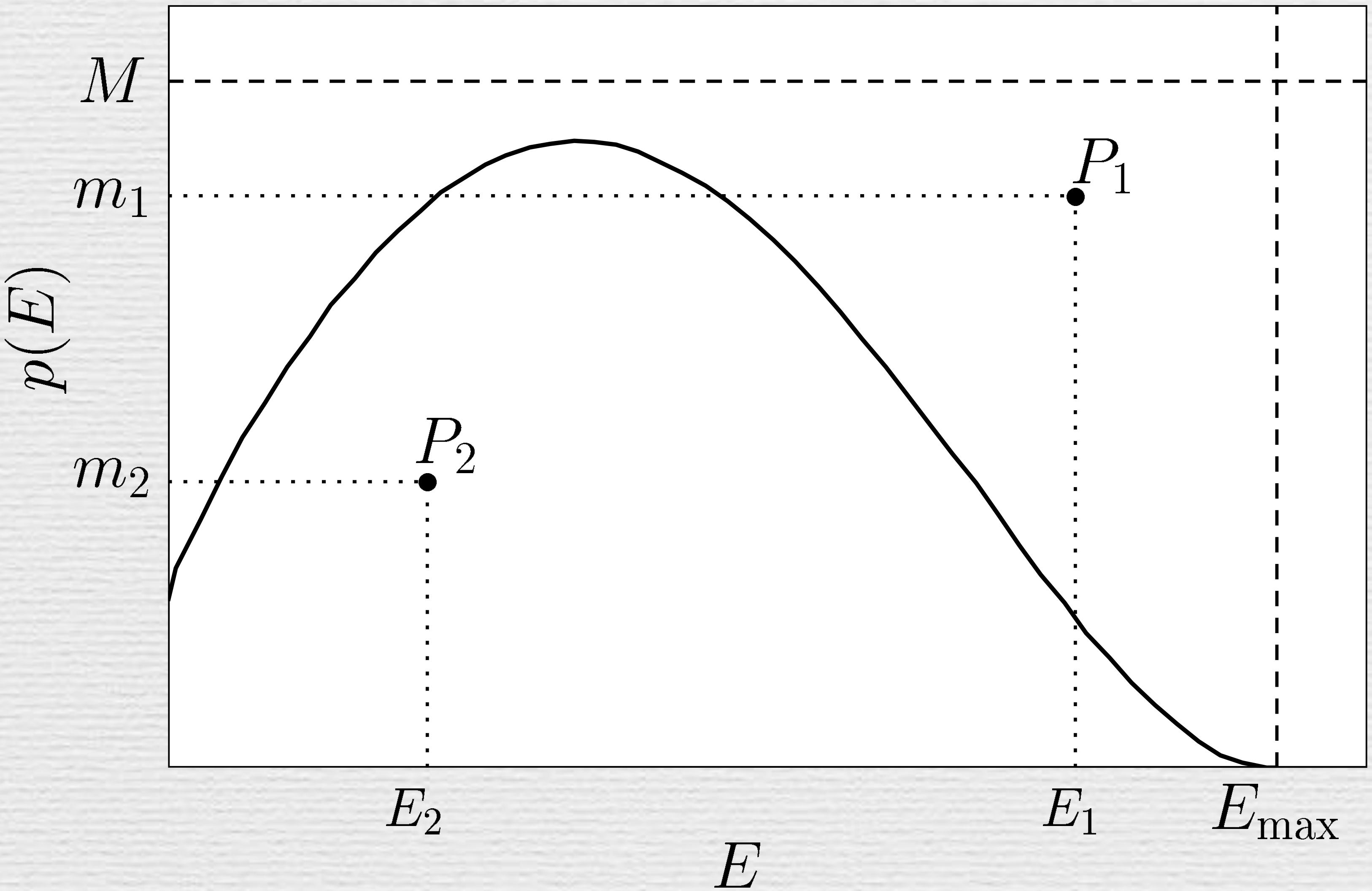


Simple exercises

Integral calculation

$$I = \int_0^{E_{\max}} \mathrm{d}E \, p(E)$$

-le us define $M \mid p(E) < M \,, \ \forall E \in [0, E_{\max}]$



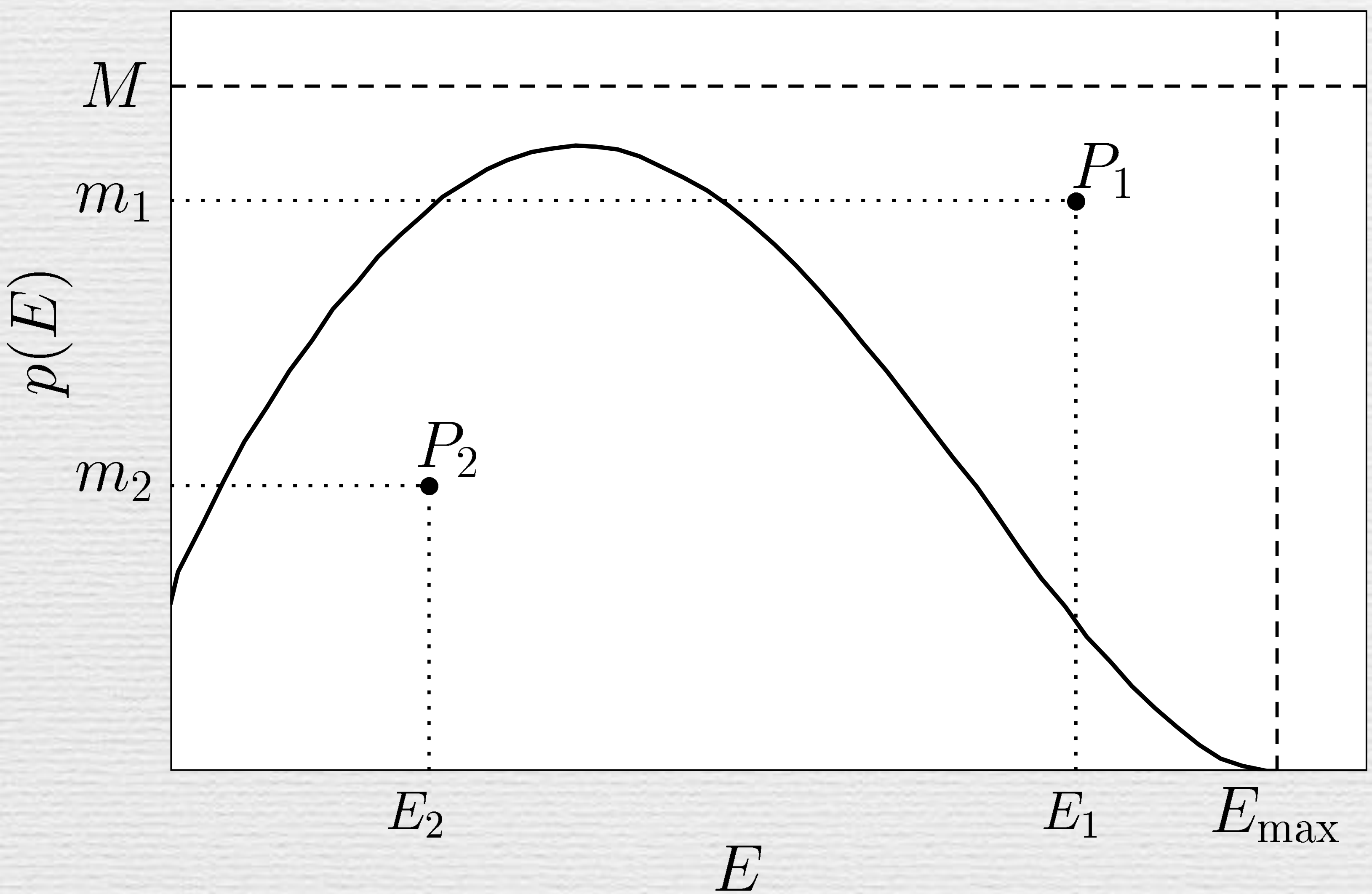
Simple exercises

Integral calculation

$$I = \int_0^{E_{\max}} \mathrm{d}E\, p(E)$$

-le us define $M \mid p(E) < M\,,\ \forall E \in [0, E_{\max}]$

-we generate $E_i \in U(0, E_{\max})\,,\ m_i \in U(0, M)$



Simple exercises

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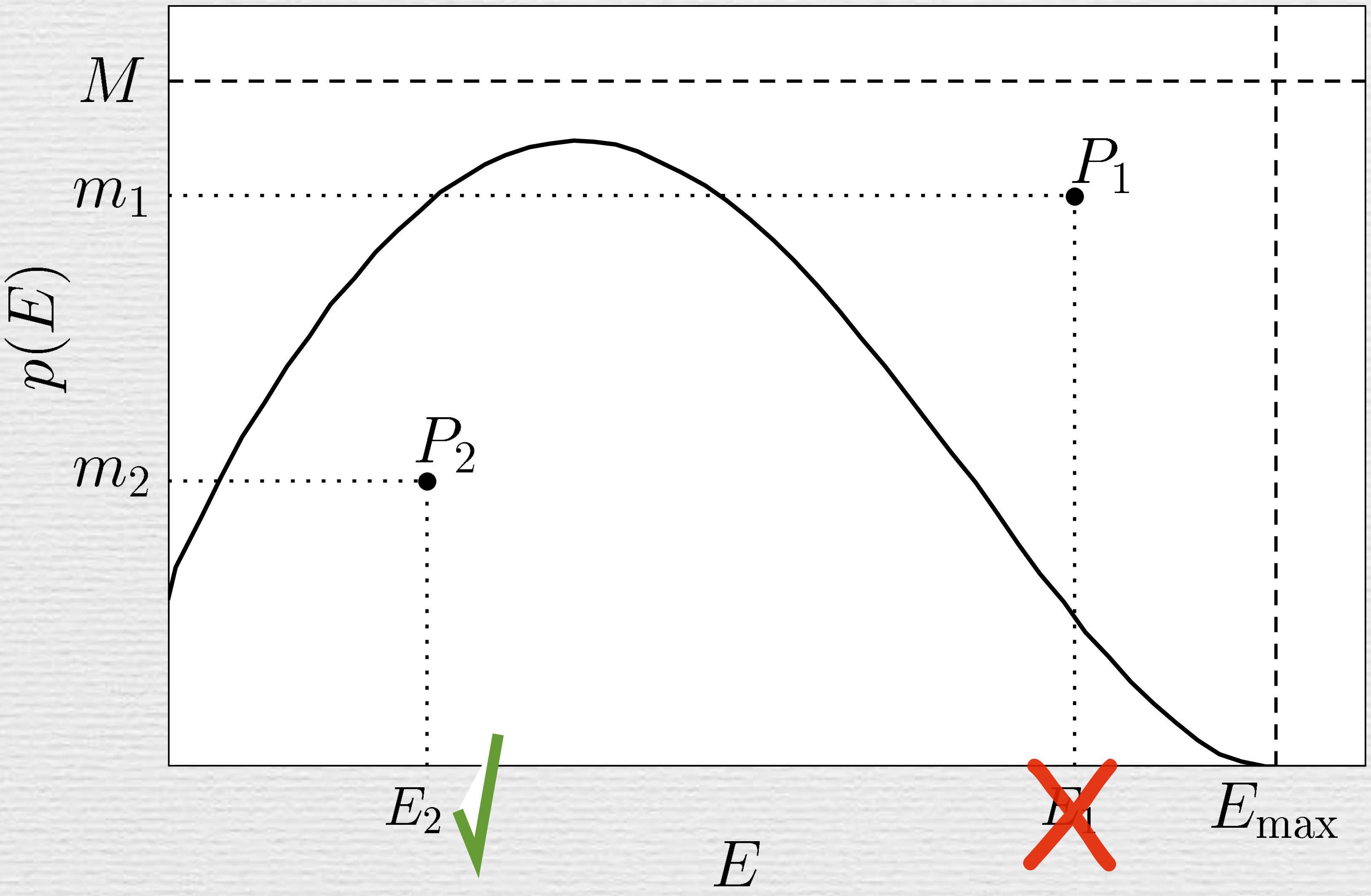


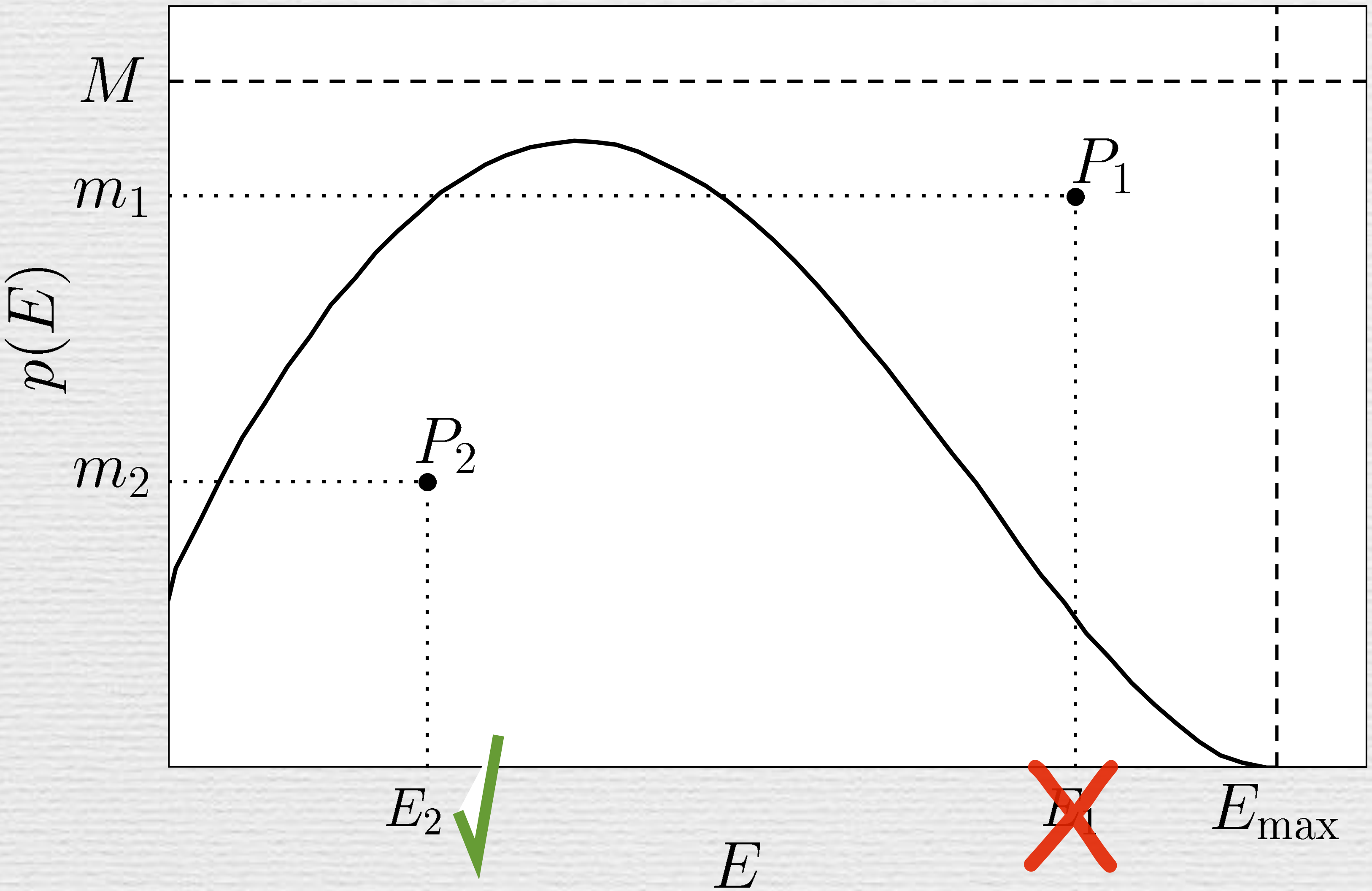
Simple exercises

Integral calculation

$$I = \int_0^{E_{\max}} \mathrm{d}E\, p(E)$$

-le us define $M \mid p(E) < M\,,\ \forall E \in [0, E_{\max}]$

-we generate $E_i \in U(0, E_{\max})\,,\ m_i \in U(0, M)$



$$I = M\, E_{\max} \left[\frac{N_{\text{int}}}{N} \pm \sigma \right]$$

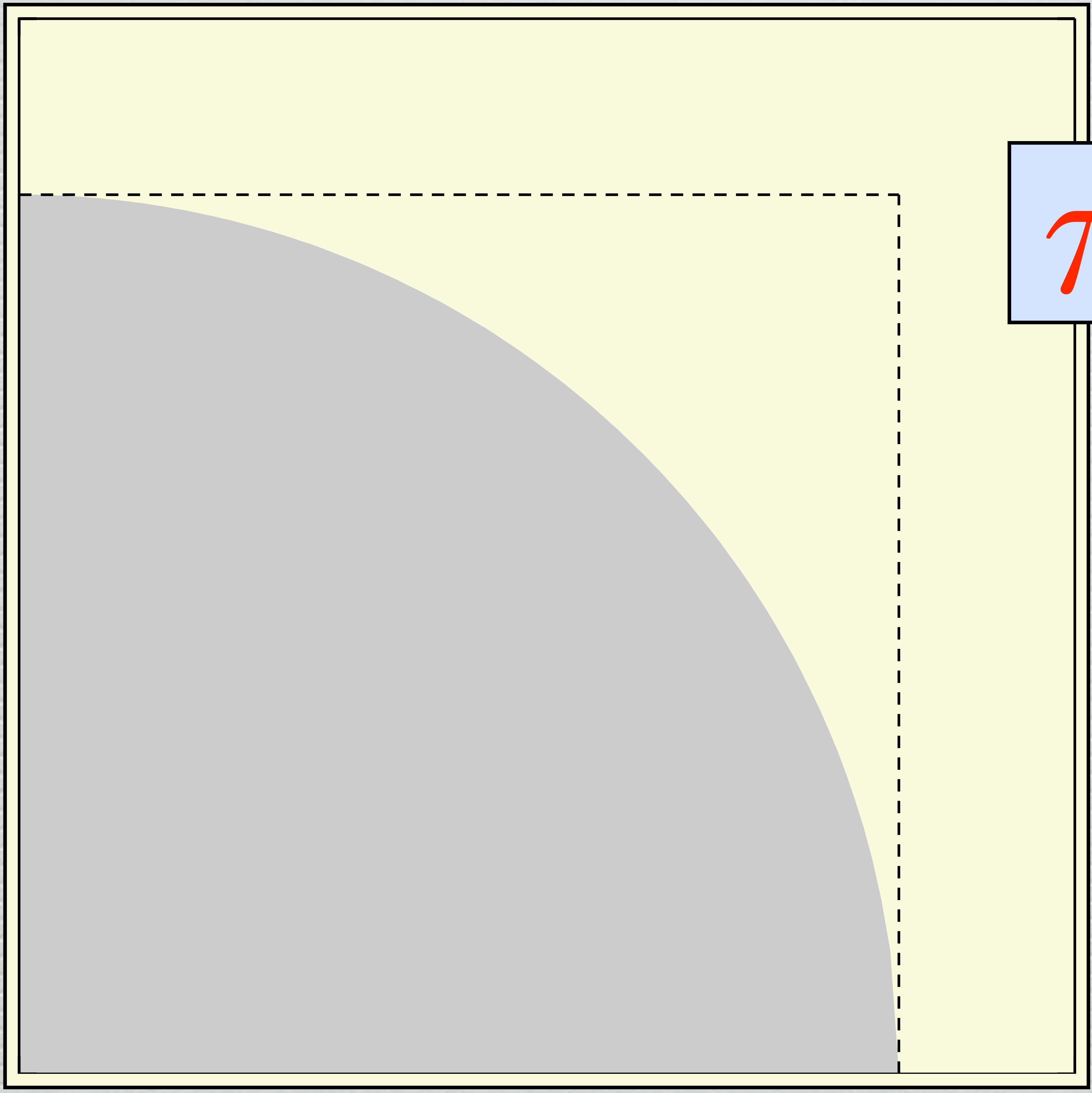
$$\sigma = \frac{1}{N} \sqrt{N_{\text{int}} \left(1 - \frac{N_{\text{int}}}{N} \right)}$$

$N_{\text{int}} \equiv$ number of interior points (e. g. P_2)

$N \equiv$ number of generated points

Simple exercises

Integral calculation: determination of π



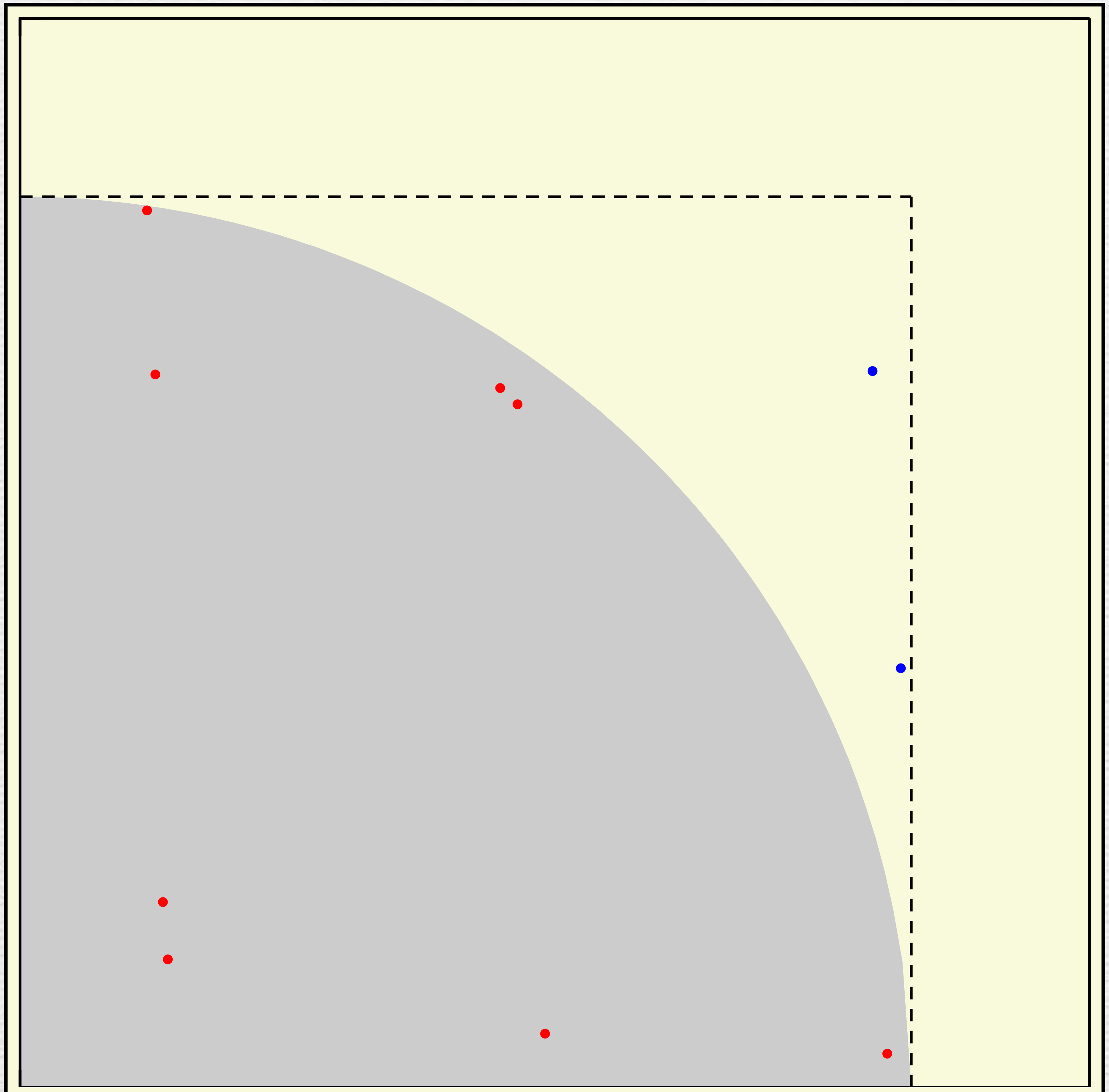
$$\pi = 4 \cdot A$$

Simple exercises

Integral calculation: determination of π

N	N_{int}	π

Integral calculation: determination of π



N	N_{int}	π
10	8	3.2 ± 0.5

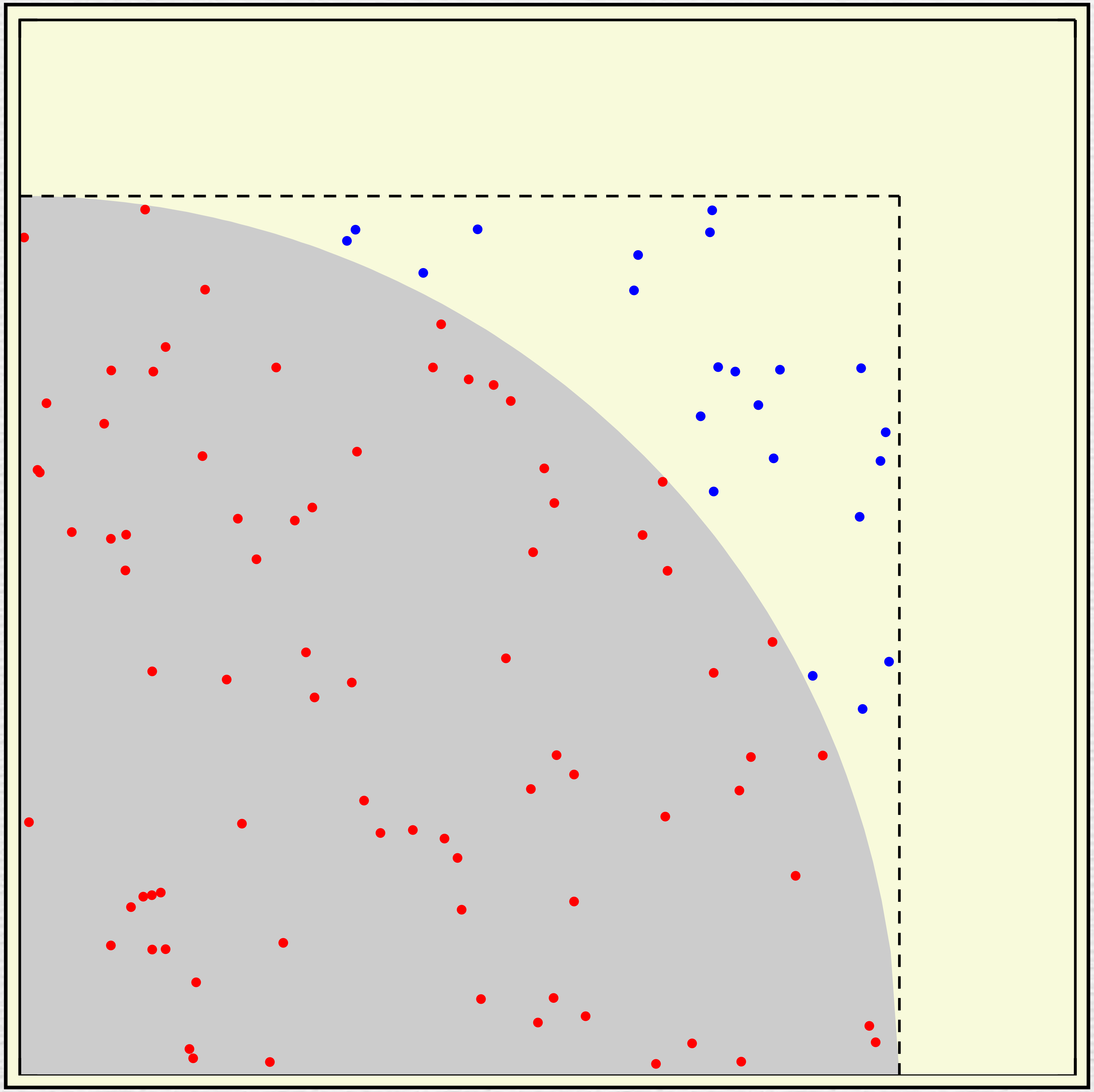
Simple exercises

Integral calculation: determination of π

N	N_{int}	π
10	8	3.2 ± 0.5

Simple exercises

Integral calculation: determination of π



N	$N_{\rm int}$	π
10	8	3.2 ± 0.5
100	78	3.12 ± 0.17

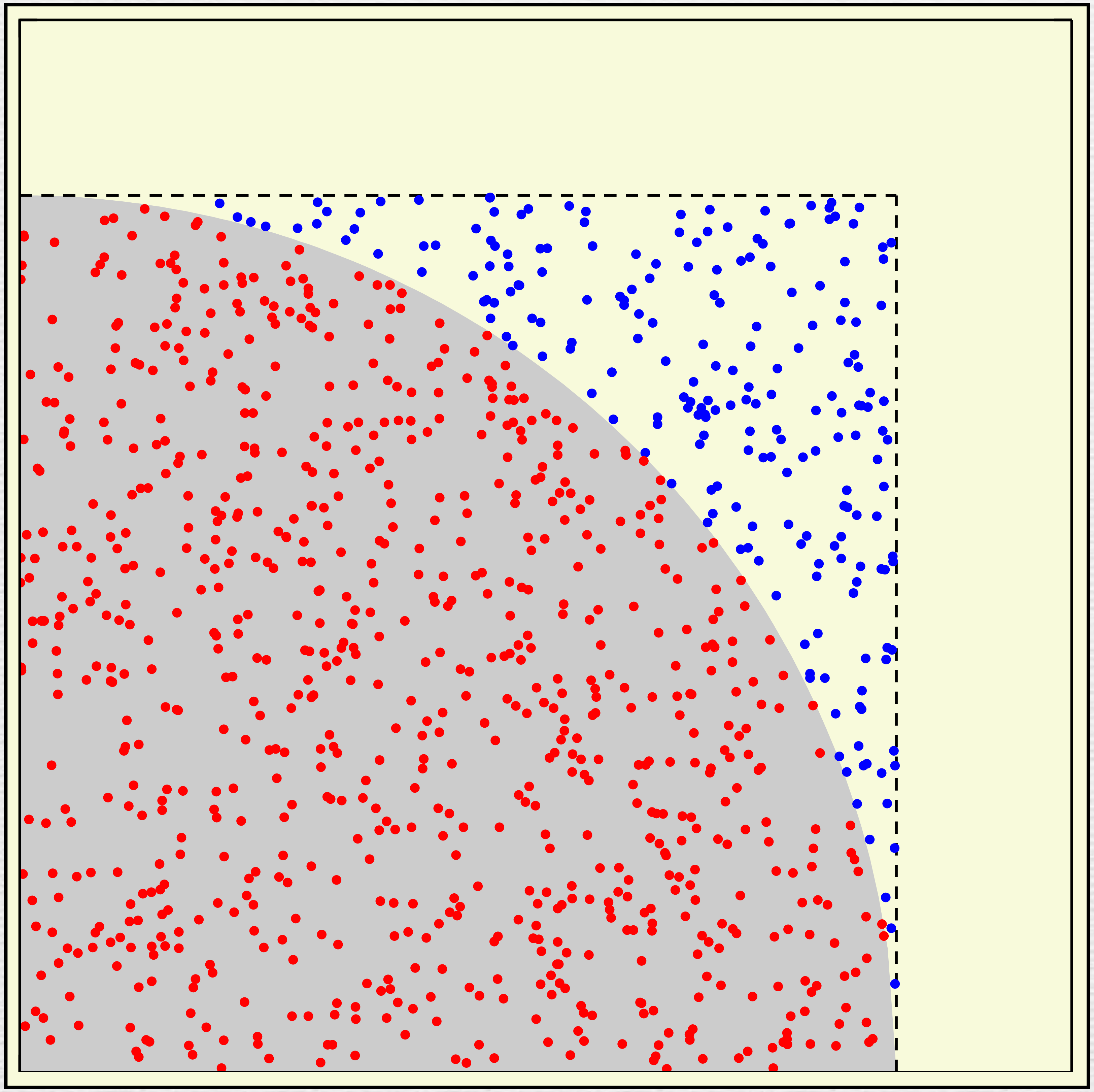
Simple exercises

Integral calculation: determination of π

N	$N_{\rm int}$	π
10	8	3.2 ± 0.5
100	78	3.12 ± 0.17

Simple exercises

Integral calculation: determination of π



N	N_{int}	π
10	8	3.2 ± 0.5
100	78	3.12 ± 0.17
1000	787	3.15 ± 0.05

Simple exercises

Integral calculation

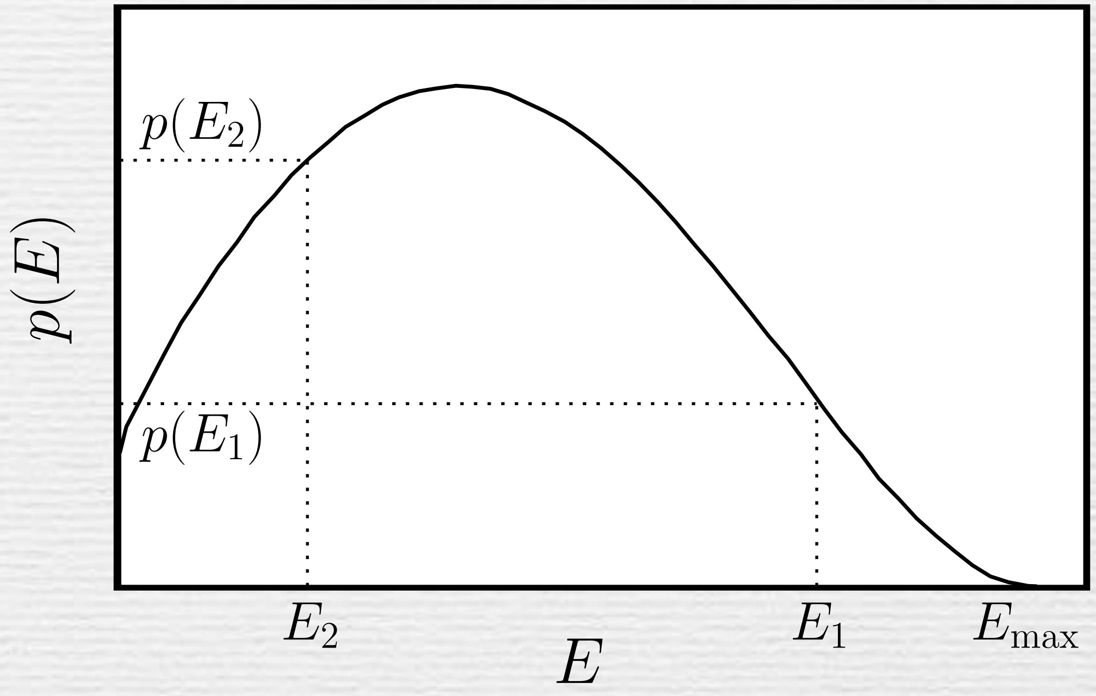
"crude" Monte Carlo method

Simple exercises

$$I = \int_0^{E_{\max}} \mathrm{d}E \, p(E)$$

Integral calculation

"crude" Monte Carlo method

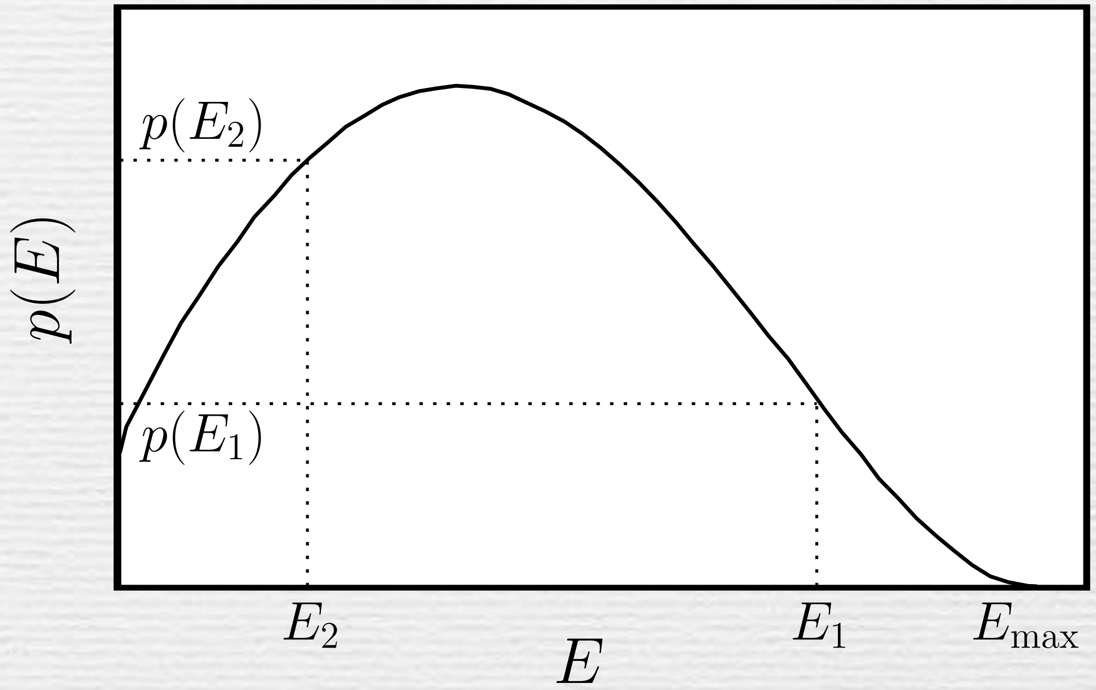


Simple exercises

$$I = \int_0^{E_{\max}} \mathrm{d}E\, p(E)$$

Integral calculation

"crude" Monte Carlo method



-we generate

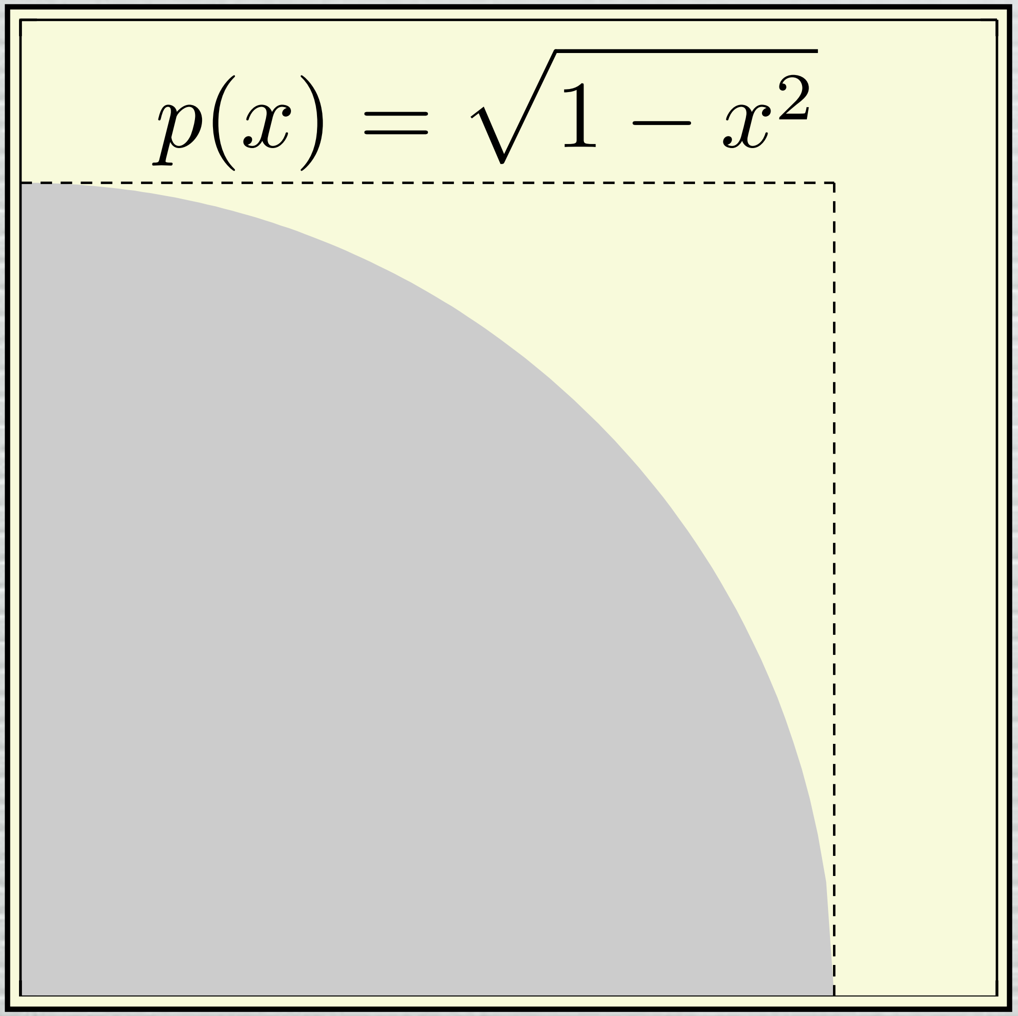
$$\{E_i \in U(0, E_{\max}),\ i = 1, \ldots, N\}$$

$$I \equiv \overline{p} = \frac{1}{N} \sum_{i=1}^{N} p(E_i)$$

$$\sigma = \frac{1}{\sqrt{N}} \left\{ \frac{1}{N} \sum_{i=1}^{N} [p(E_i)]^2 - \overline{p}^2 \right\}^{1/2}$$

Simple exercises

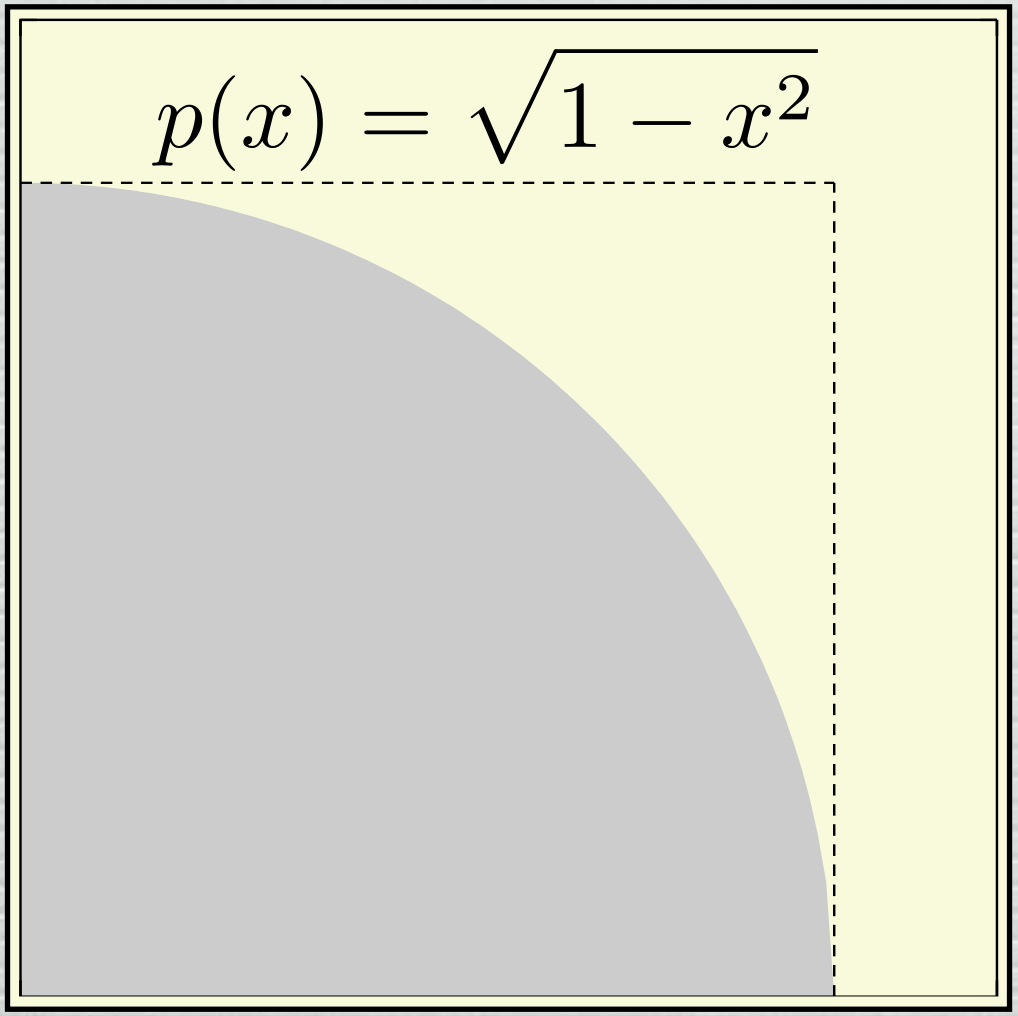
Integral calculation: determination of π



$$\boxed{\pi = 4 \cdot A}$$

Simple exercises

Integral calculation: determination of π



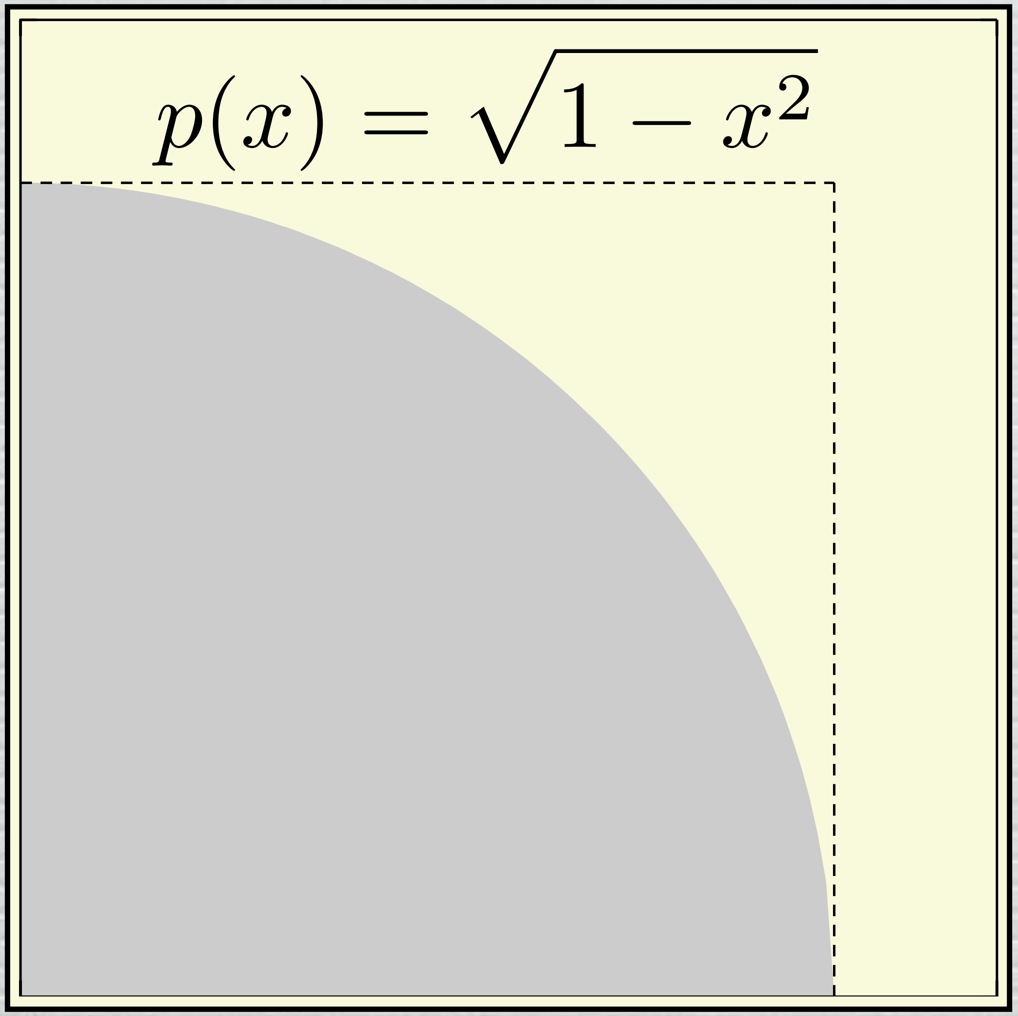
-we generate

$$\{x_i \in U(0,1),\ i = 1, \ldots, N\}$$

$$\pi = 4 \cdot A$$

Simple exercises

Integral calculation: determination of π



-we generate

$$\{x_i \in U(0,1),\ i = 1, \ldots, N\}$$

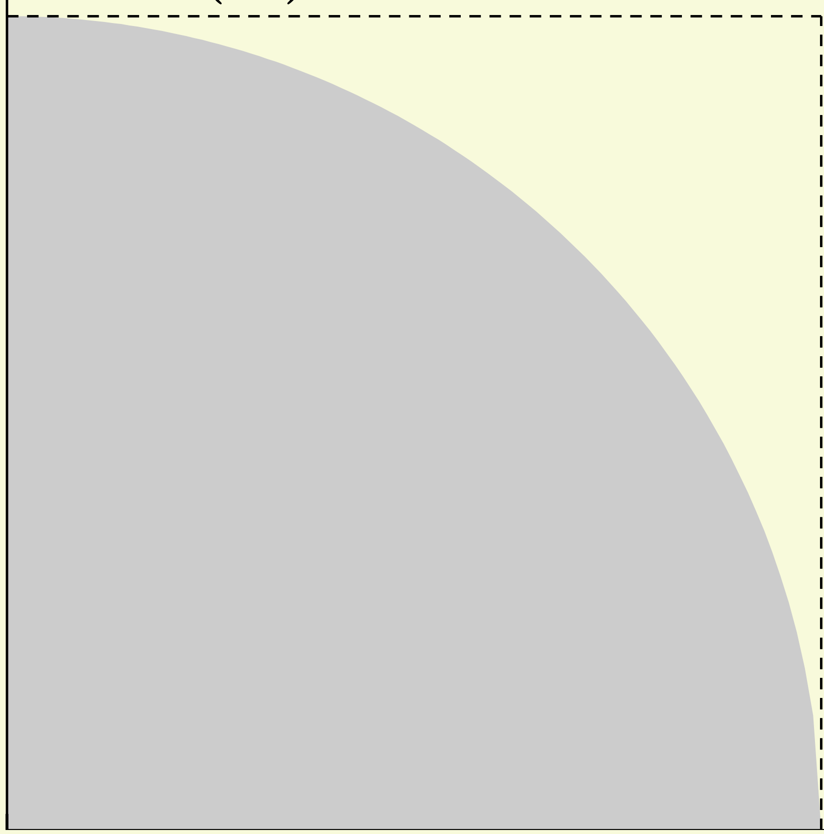
$$I = \frac{1}{N} \sum_{i=1}^{N} \sqrt{1 - x_i^2}$$

$$\pi = 4 \cdot A$$

Simple exercises

Integral calculation: determination of π

$$p(x) = \sqrt{1 - x^2}$$



-we generate

$$\{x_i \in U(0,1),\ i = 1, \ldots, N\}$$

$$I = \frac{1}{N} \sum_{i=1}^{N} \sqrt{1 - x_i^2}$$

	N_{int}	π
10	8	3.2 ± 0.5
100	78	3.12 ± 0.17
1000	787	3.15 ± 0.05

N	π
10	3.4 ± 0.2
100	3.18 ± 0.09
1000	3.13 ± 0.03

$$\pi = 4 \cdot A$$

Simple exercises

Queue dynamics

-a simple problem: medical consultation

Problem: we want studying how the number of patients waiting in a medical consultation behaves and analyze possible strategies to proceed in the better (or not) way

-determine the number of waiting patients in each moment

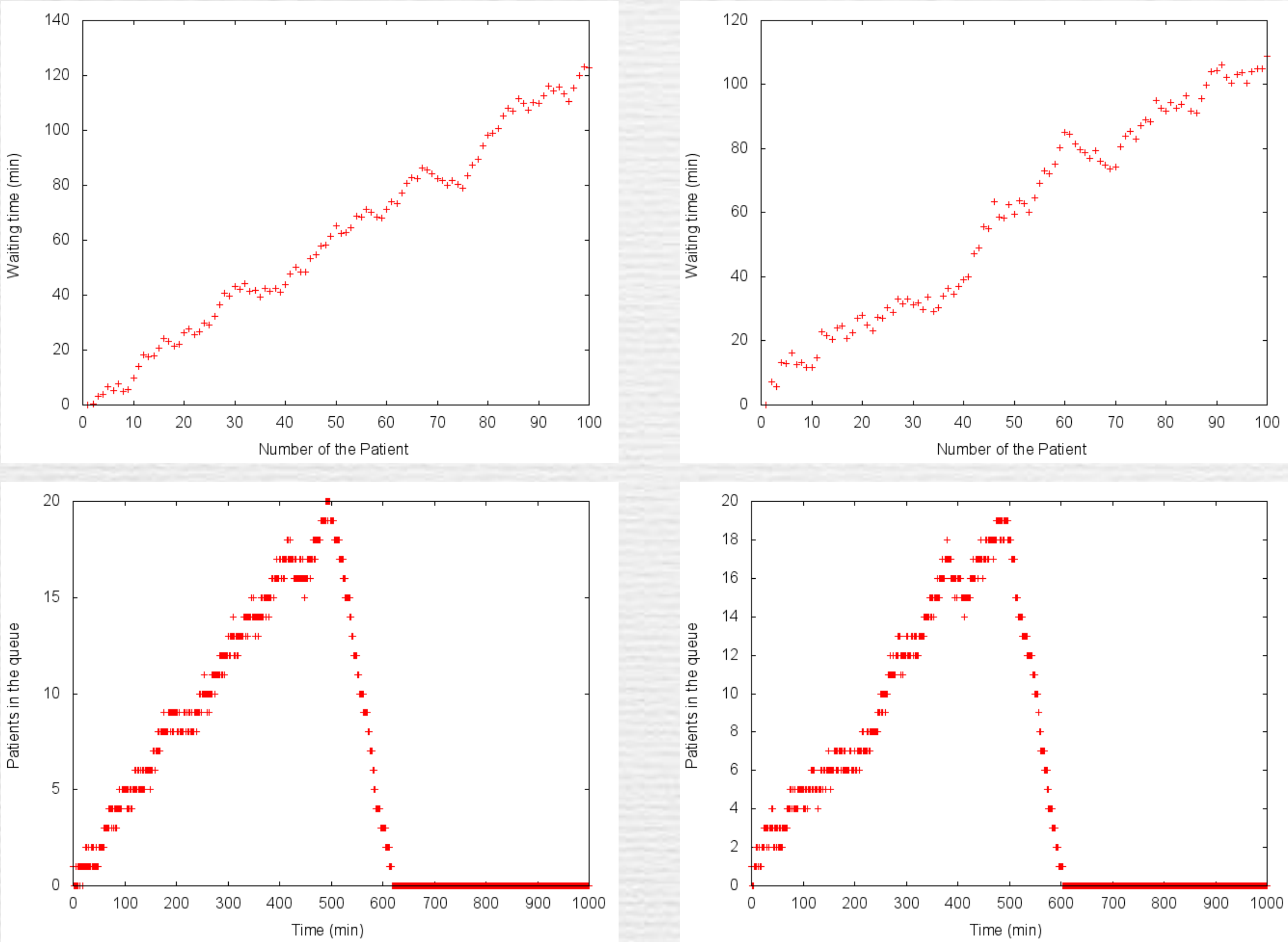
-determine the waiting time of each of them

Ingredients:

- N_p patients appointed each t_{app} minutes
- consultation time: t_c sample in a given PDF

U(2 min, 10 min)   N(5 min, 1 min)

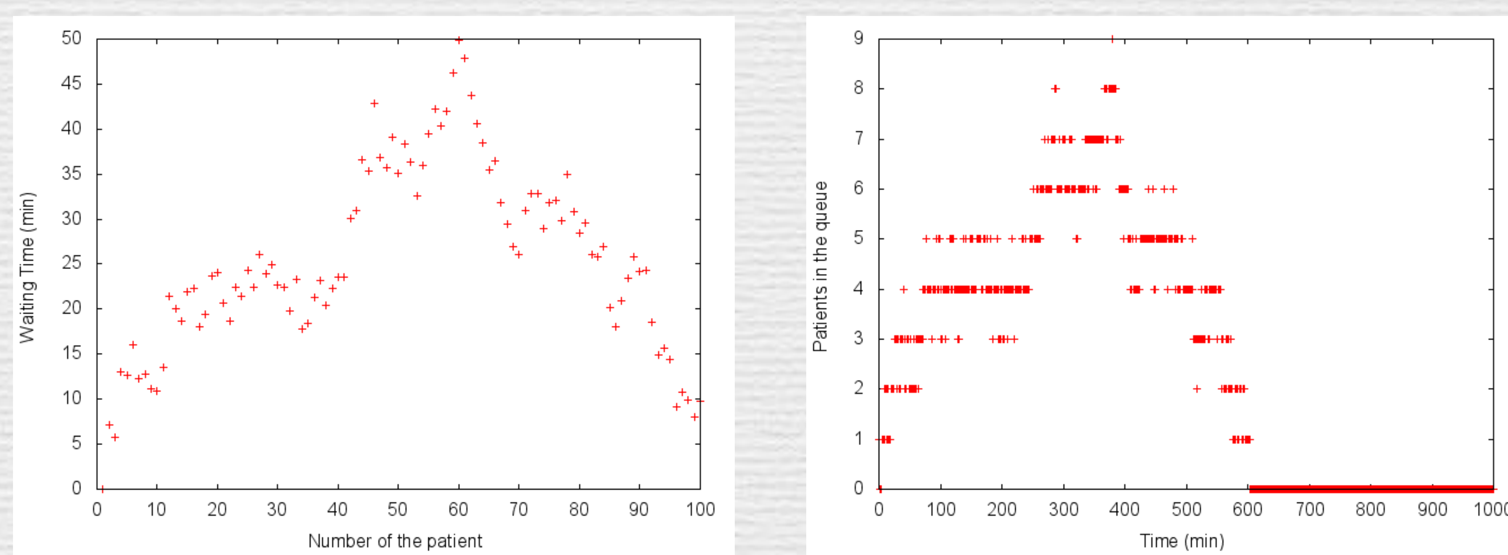
t_{app} = 5 min



Waiting time for each patient (upper panels) and queue length as a function of time (lower panels) found for the uniform (left panels) and Gaussian (right panels) distributions.

N(5 min, 1 min)

t_{app} + 1 min * n



Waiting time for each patient (left panel) and queue length as a function of time (right panel) obtained for the Gaussian distribution with the modified appointment schedule.

Thanks for the attention