SCHEDULE TODAY

- Reminder deadline
- Recap MC
- Dirac delta function as initial condition applied to diffusion equation
- Gaussian distributed random numberes
- Random walk:
- Brownian motion/Wiener process
- Ornstein Uhlenbeck process

REMINDER DEADLINE

- 13/5/2026: final in-class test.

Important to complete all weekly exercises, since it will allow you to reuse some of the code.

RECAP

MC INTEGRATION WITH ERROR ESTIMATION

An integral $F = \int_0^L f(x)dx$ can be calculated by the interval of the integral L times the average of the function to be integrated over the interval $\langle f \rangle$. The sample points are N uniform random numbers inside the interval $[0, L]$ and the resulting estimate for the integral $\pm$ 1 standard deviation is

$$F \approx L\langle f\rangle_N \pm L\sqrt{\frac{1}{N}\left(\langle f^2\rangle_N - \langle f\rangle_N^2\right)}$$

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$$F \approx L\langle f \rangle_N \pm L\sqrt{\frac{1}{N}\left(\langle f^2 \rangle_N - \langle f \rangle_N^2\right)}$$

INTEGRATING $f(x) = x^2$ FROM 0 TO 1.

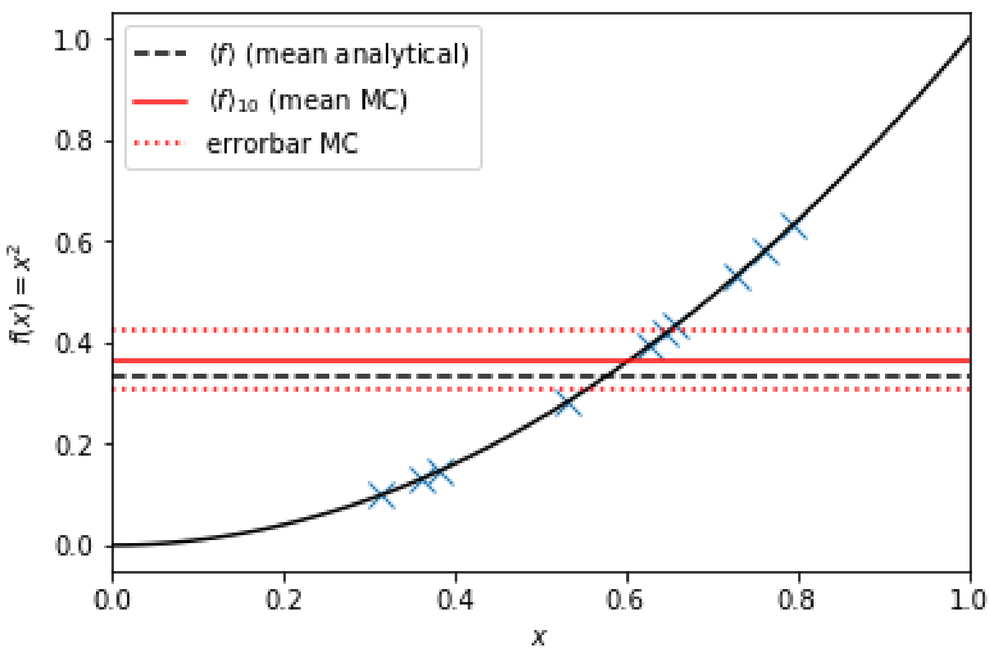
Python code:

```
import numpy as np
# Function to integrate
def f(x):
    return x**2

# Generate the random numbers from a uniform distribution
a, b = 0, 1
nsamples = 10
X=np.random.uniform(a, b, nsamples)

# Value of integral
mean_f=np.mean(f(X))
F=(b-a)*mean_f
```

Analytical result: $F = \frac{1}{3}x^3\Big|_0^1 = 1/3.$



$\langle f \rangle$ (mean analytical)
$\langle f \rangle_{10}$ (mean MC)
errorbar MC
$f(x) = x^2$
x

DIFFUSION EQUATION (2)

Let us now return to the diffusion equation:

$$\frac{\partial u(t, \mathbf{r})}{\partial t} = \alpha \nabla^2 u(t, \mathbf{r})$$

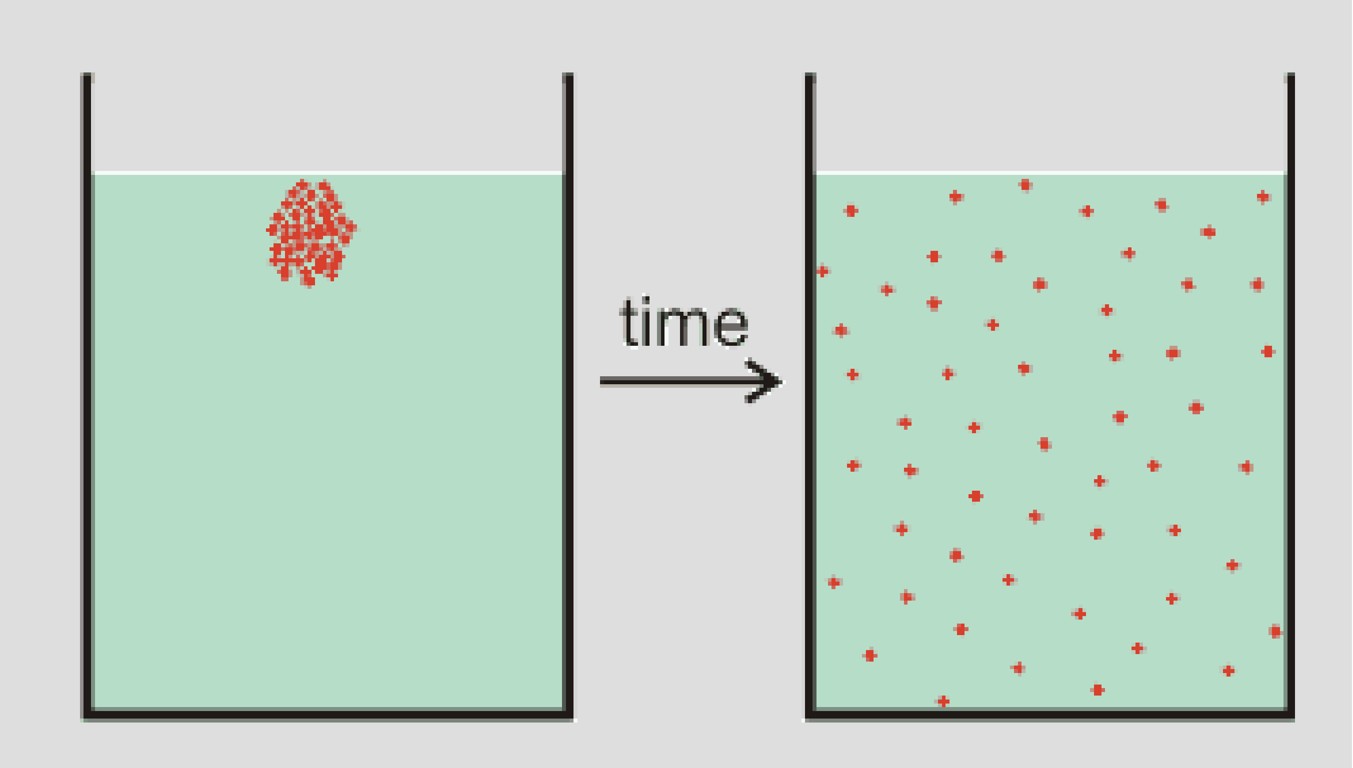
Then in one spatial dimension this diffusion equation reduces to

$$\frac{\partial u(t, x)}{\partial t} = \alpha \frac{\partial^2 u(t, x)}{\partial x^2}$$

The diffusion equation can be used to model heat diffusion or diffusion of particles in a quiescent flow

INK DIFFUSION

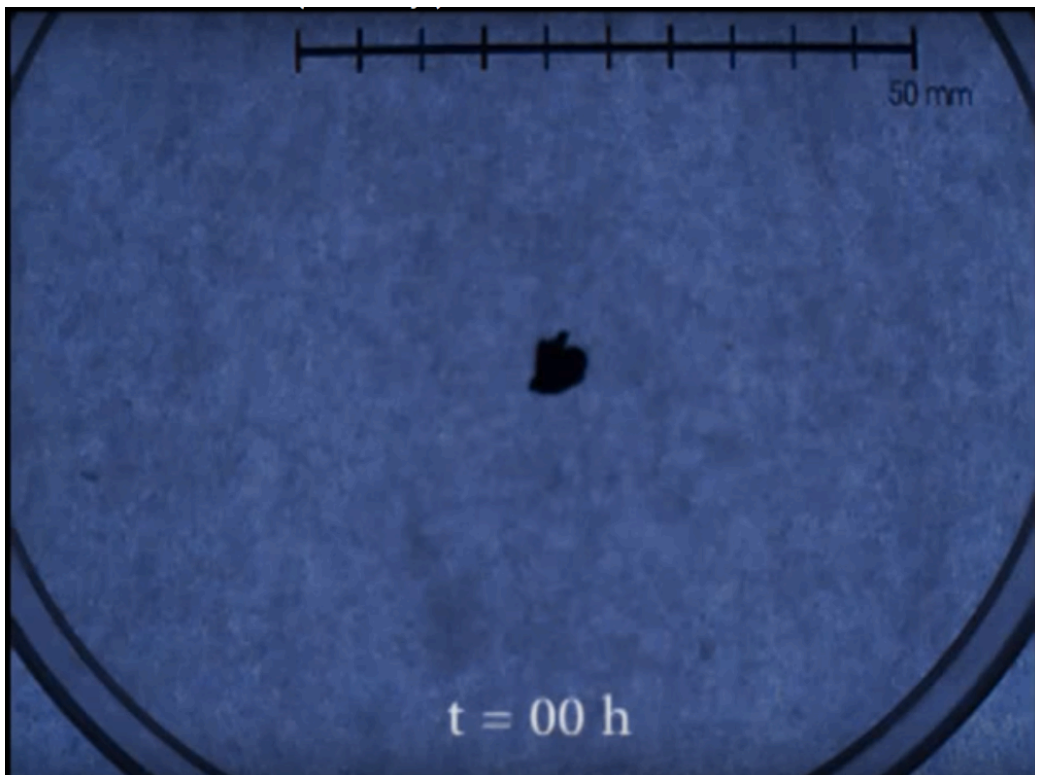
Heat diffusion similar to a ink diffusing in quiescent water (without convection)



EXPERIMENTAL SYSTEM

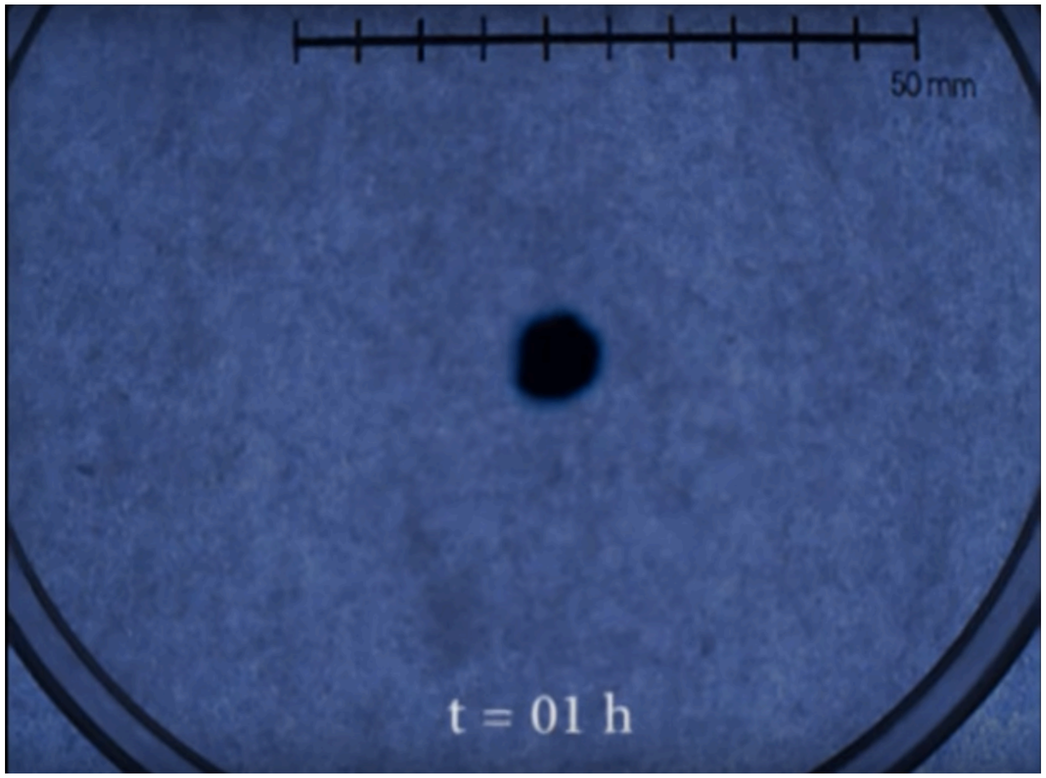
Insert ink at $t = 0$ inside a jelly matrix

[//]: # (Experiment conducted at McMaster University, Department of Material Science and Engineering)

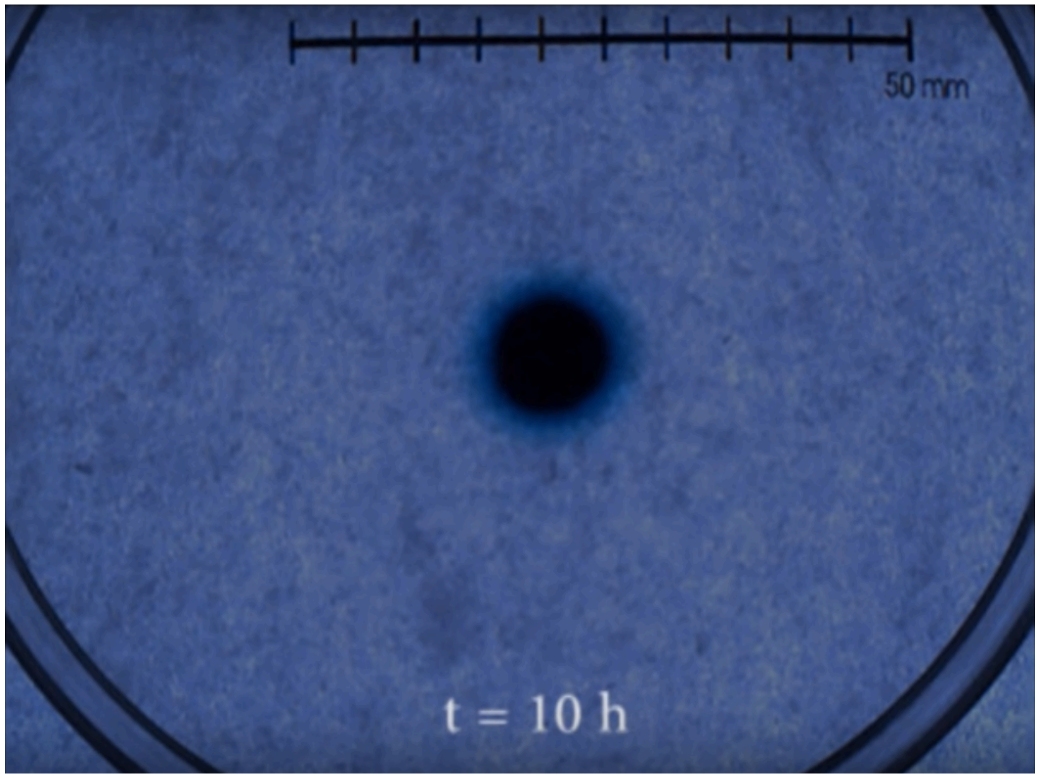


https://www.youtube.com/watch?v=6zysNwl6Zuo

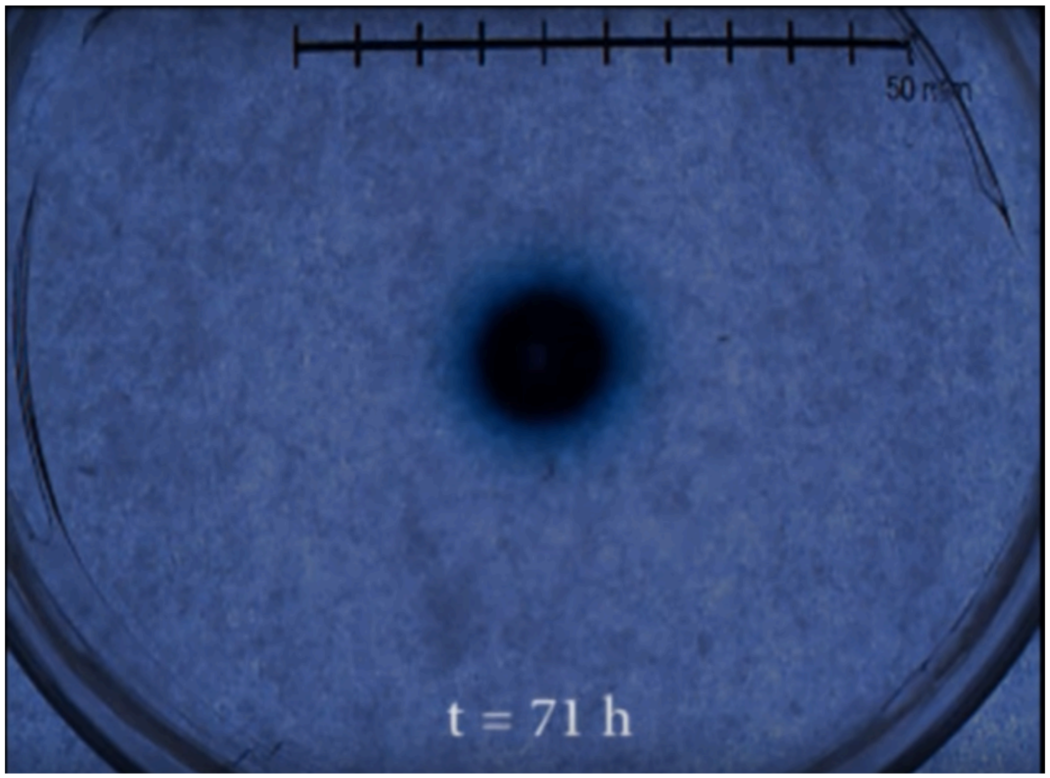
Ater one hour



After 10 hours



After 71 hours



HOW TO SOLVE INK DIFFUSION NUMERICALLY?

INITIAL CONDITION: DELTA FUNCTION

The ink diffusion can be modelled by considering another initial condition for the diffusion equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

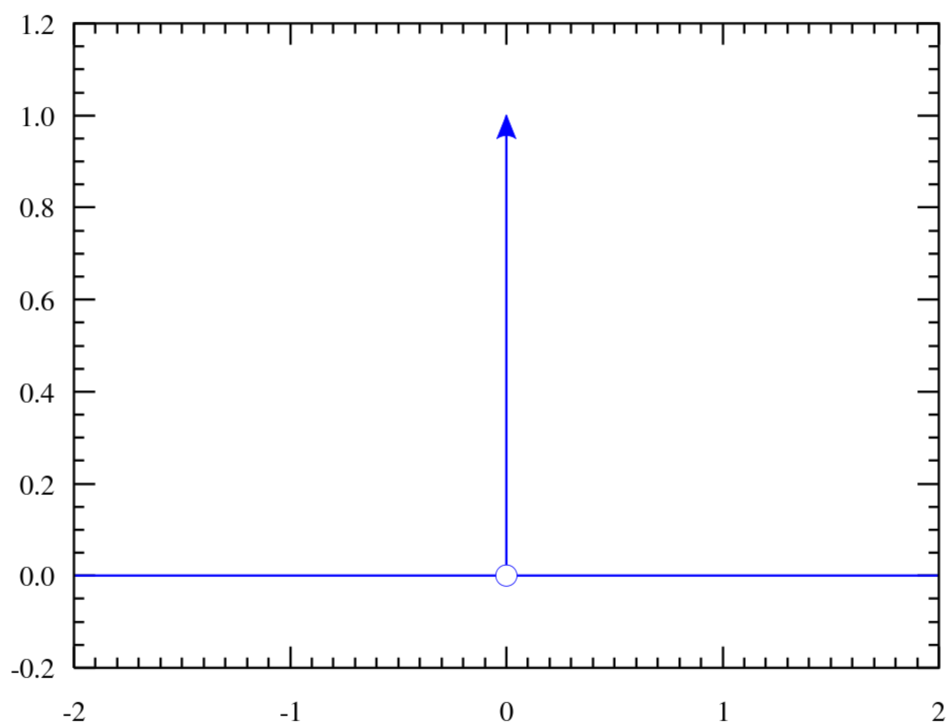
namely

$$u(0, x) = \delta(x - x_M)$$

(M for middle) and take boundary conditions $u(t, x_L) = u(t, x_R) = 0$.

DEFINITION DELTA FUNCTION

The **Dirac delta function** $\delta(x - x_0)$ is a function peaked near $x = x_0$ and zero otherwise



AREA

The peak is constructed in such a way, that the area of the delta function is finite, and equal to 1:

$$\int_{-\infty}^{\infty} \delta(x)dx = 1$$

SIFTING PROPERTY

An important property of the Dirac delta function is the **sifting property**:

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_0)dx = f(x_0)$$

So the integral of a function multiplied by the delta function is just the function itself at where the delta function peaks.

INTUITIVE DERIVATION SIFTING PROPERTY

- The delta function is zero away from x_0, so the function multiplied by 0 gives 0. Hence the integration can be confined to a region close to x_0, where the delta function is strongly peaked:

$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)dx = \int_{x_0-\Delta}^{x_0+\Delta} f(x)\delta(x-x_0)dx$$

- For x near x_0 the function $f(x)$ is just $f(x_0)$:

$$\int_{x_0-\Delta}^{x_0+\Delta} f(x)\delta(x-x_0)dx = \int_{x_0-\Delta}^{x_0+\Delta} f(x_0)\delta(x-x_0)dx$$

- $f(x_0)$ is a constant, so can be taken in front of the integral

$$\int_{x_0-\Delta}^{x_0+\Delta} f(x_0)\delta(x-x_0)dx = f(x_0)\int_{x_0-\Delta}^{x_0+\Delta} \delta(x-x_0)dx$$

- The area of the delta function is 1, so

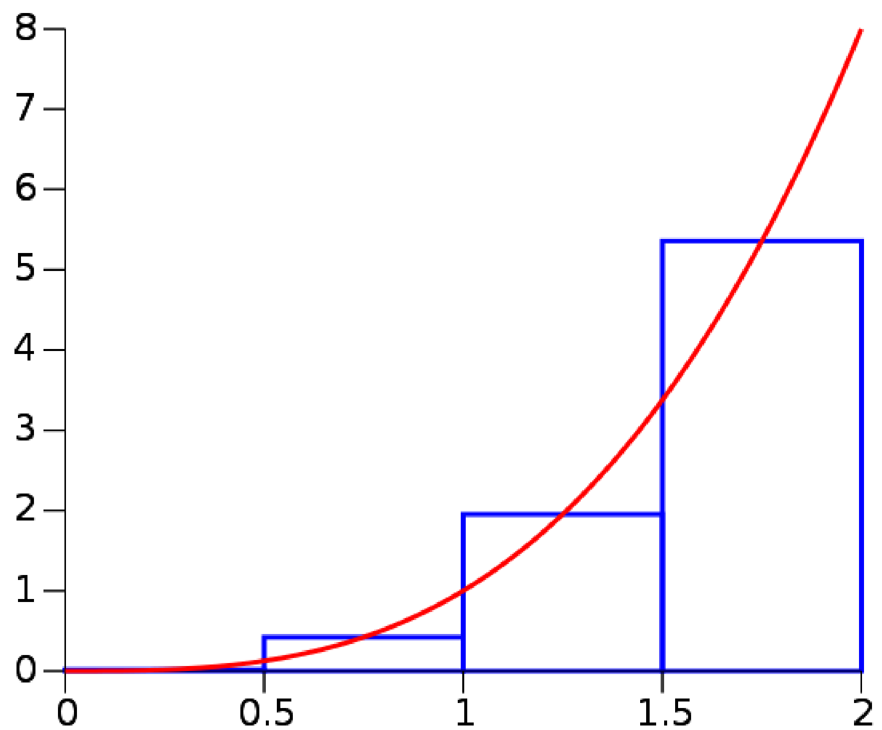
$$f(x_0)\int_{x_0-\Delta}^{x_0+\Delta} \delta(x-x_0)dx = f(x_0)$$

HOW TO INCORPORATE THE DELTA FUNCTION IN A FINITE DIFFERENCE SCHEME?

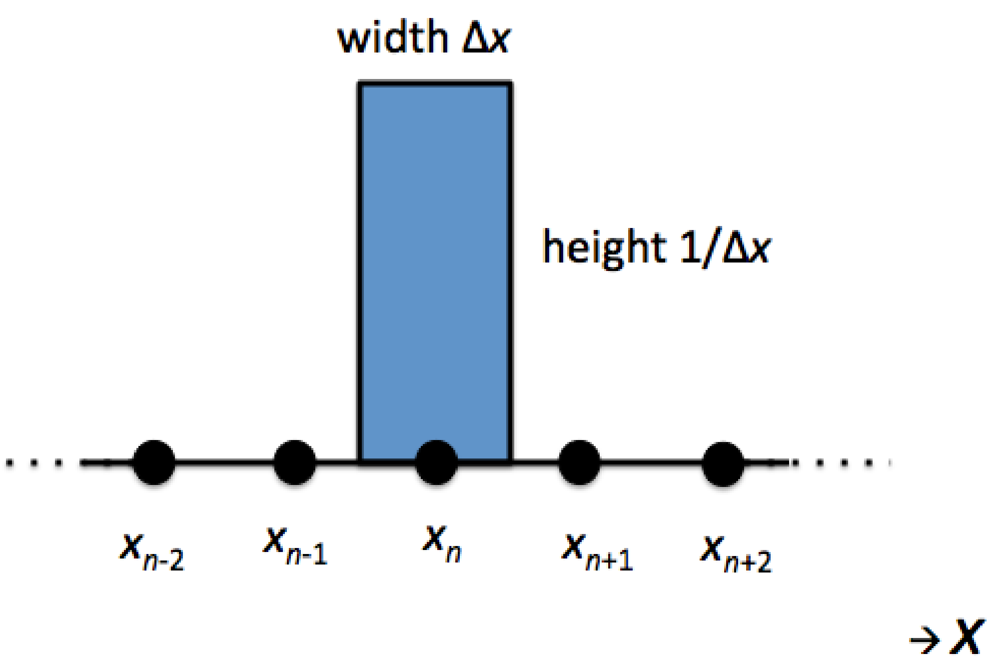
In a finite difference scheme integrals are replaced by sums:

$$\int u(t,x)dx \approx \sum_n u(t,x_n)\Delta x$$

just like the solution of a first order differential equation using, e.g., the *Euler method*, or the *midpoint method*.



The area of a delta function is 1, so set the height of the peak such that the area becomes 1:



Assume that the middle is at x_n, $x_M = x_n$, then

$$\int u(t=0,x)dx = \int \delta(x - x_M)dx = 1$$
$$\approx u(x_n)\Delta x = 1$$

Hence the incorporation of a delta function as a condition can be established by setting

$$\boxed{u(x_n) = \frac{1}{\Delta x}}$$

RESULTS EULER FORWARD FOR DIFFUSION EQUATION WITH DELTA FUNCTION AS INITIAL CONDITION

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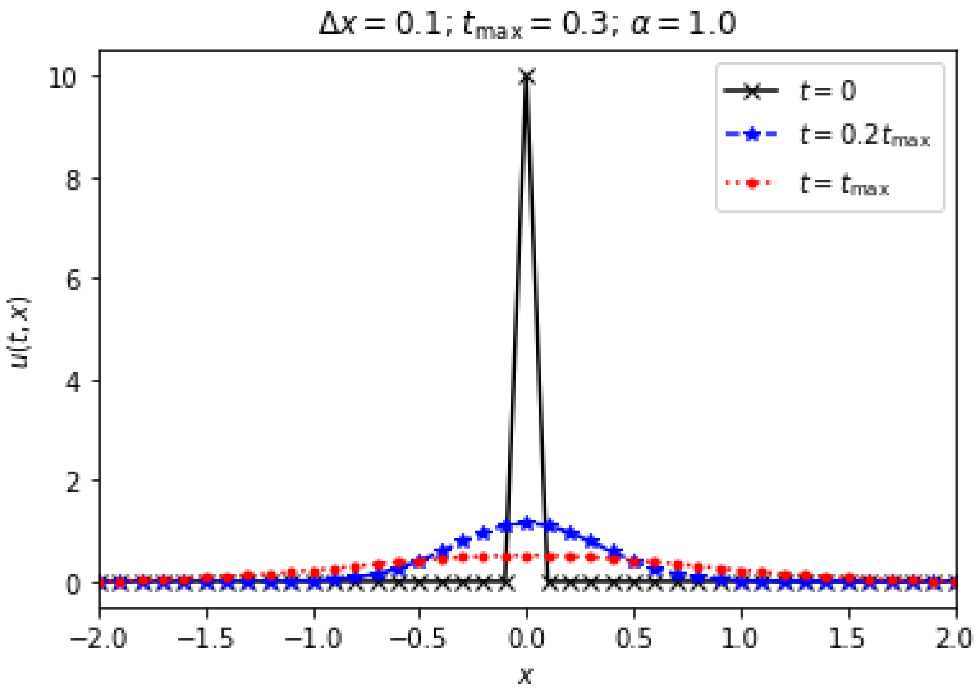
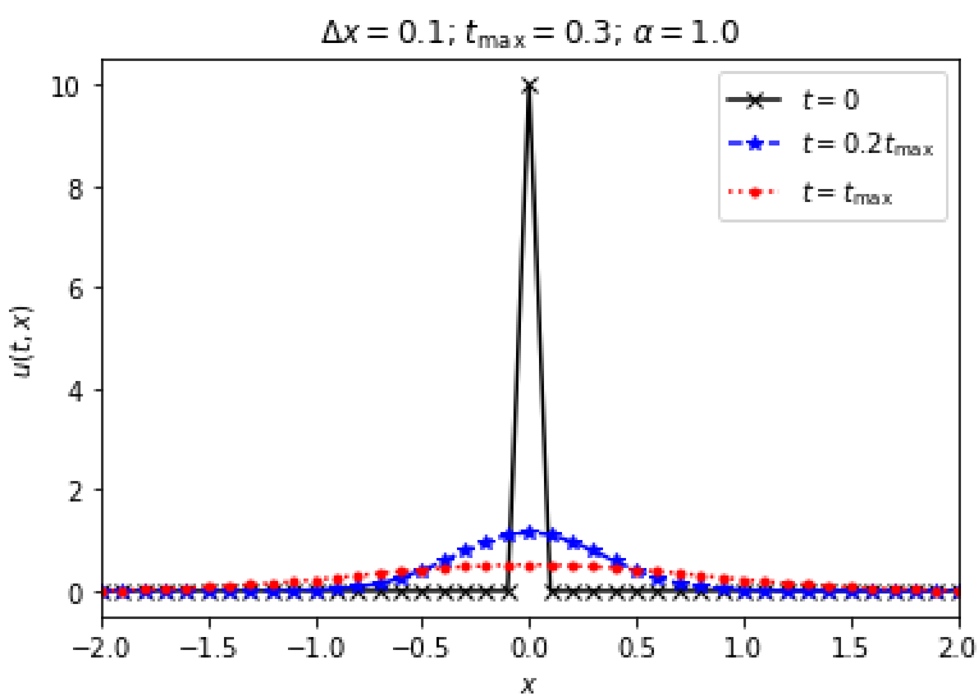

$\Delta x = 0.1$; $t_{\max} = 0.3$; $\alpha = 1.0$
$t = 0$
$t = 0.2t_{\max}$
$t = t_{\max}$
$u(t, x)$
x
10
8
6
4
2
0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

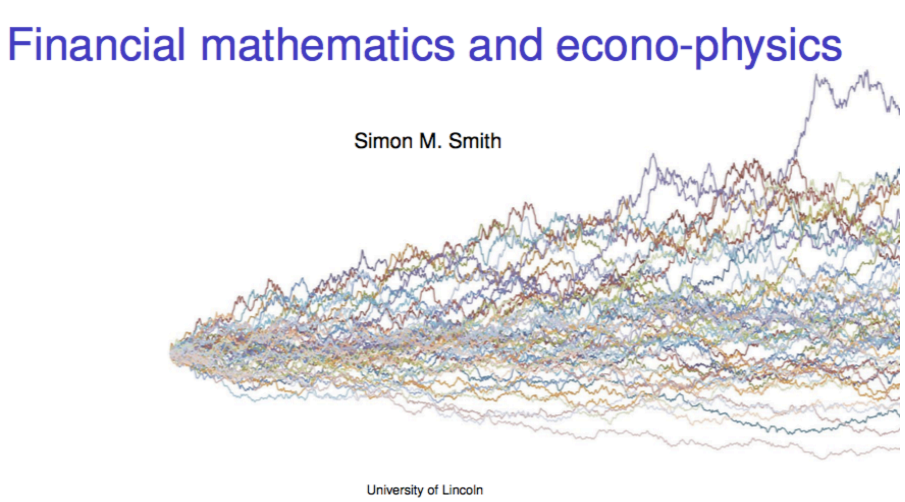


Notice that at $t = 0$ the peak is at 10. Together with $\Delta x = 0.1$, this makes the area equal to $10 \times 0.1 = 1$.

STOCHASTIC PROCESSES

The diffusion equation is similar to Brownian motion.

- Heat diffusion: particles bounce against each other thereby transferring kinetic energy and hence heat.
- Order of 10^{23} particles per gram: the diffusion equation is an *average description* and suffices for heat diffusion.
- Alternative: model a *single* particle. The particle will be kicked around by other particles: Brownian motion.
- Similar to second year module: financial mathematics and econo-physics. It would be good to revise Simon's lecture notes.



RANDOM VARIABLE

Let us first introduce some notation.

$Z \sim \mathrm{Norm}(\mu, \sigma^2)$: This notation with the tilde means Z is a random variable, which has a normal (i.e., Gaussian, so bell-shaped curve) probability density function with mean μ and variance σ^2 (and hence standard deviation σ).

MULTIPLICATION OF RANDOM VARIABLE WITH CONSTANT

Note: if

$$Z \sim \mathrm{Norm}(\mu, \sigma^2)$$

then

$$kZ \sim \mathrm{Norm}(k\mu, k^2\sigma^2)$$

for a constant $k > 0$.

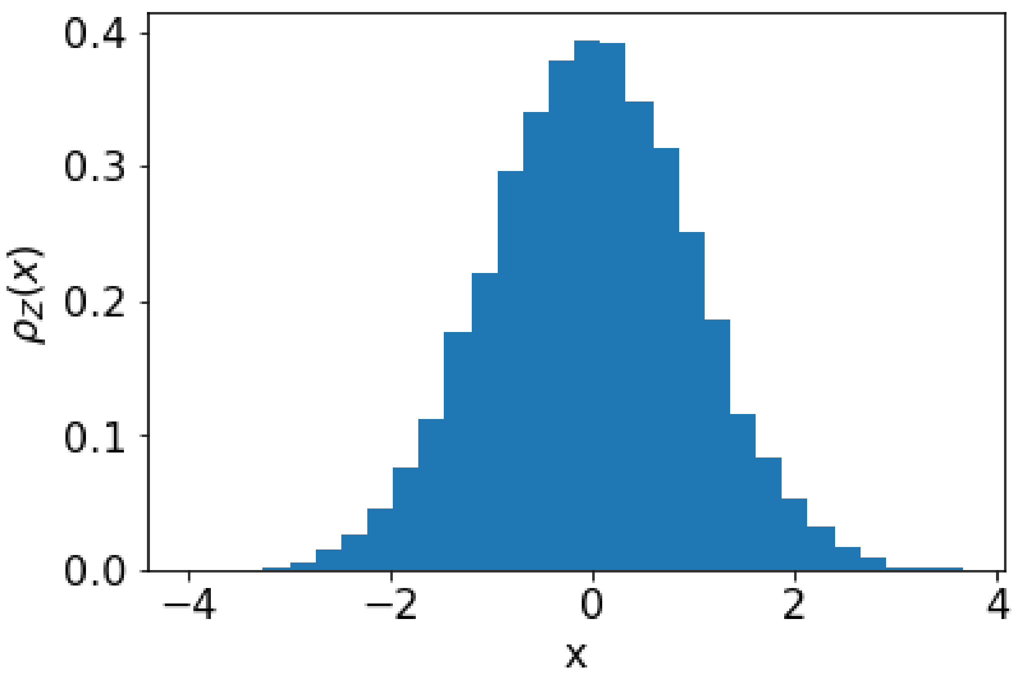
Hence if one has a random variable with a standard deviation of 1, a new random variable with standard deviation of k can be constructed by multiplying it by k.

GAUSSIAN DISTRIBUTED RANDOM NUMBERS

PYTHON

In python n normally distributed random variables Z_i with zero mean, $\mu = 0$, and unit variance, $\sigma^2 = 1$ can be generated by

```
import numpy as np
import matplotlib.pyplot as plt
mu, sigma = 0, 1                        # mean and standard deviation
n = 10000                               # number of random numbers
Z_all=np.random.normal(mu, sigma, n)    # Generate the random numbers
plt.hist(Z_all, 30, density=True)       # Show a histogram of 30 bins
```


0.4
0.3
0.2
0.1
0.0
$\rho_Z(x)$
−4
−2
0
2
4
x

DISCRETE RANDOM WALK

After every time step the person takes a unit step in a random direction.

WIENER PROCESS

A continuous-time equivalent of a random walk is given by the Wiener process, $W(t)$.

Definition: **Brownian motion**, also known as the **Weiner process**: a *continuous* time-dependent random process such that for all times $0 \leq s < t$:

1. $W(0) = 0$; the process starts at the origin.
2. $W(t) - W(s)$ is normally distributed with mean 0 and variance $t - s$, i.e., $W(t) - W(s) \sim \mathrm{Norm}(0, t - s)$.
3. $W(t) - W(s)$ is independent of $W(u)$ for all times $u \leq s$; increments are independent.

In particular, substituting $s = 0$ in property 2 gives that $W(t)$ is normally distributed with mean 0 and variance t, $W(t) \sim \mathrm{Norm}(0, t)$. Or, in other words, the probability density function is

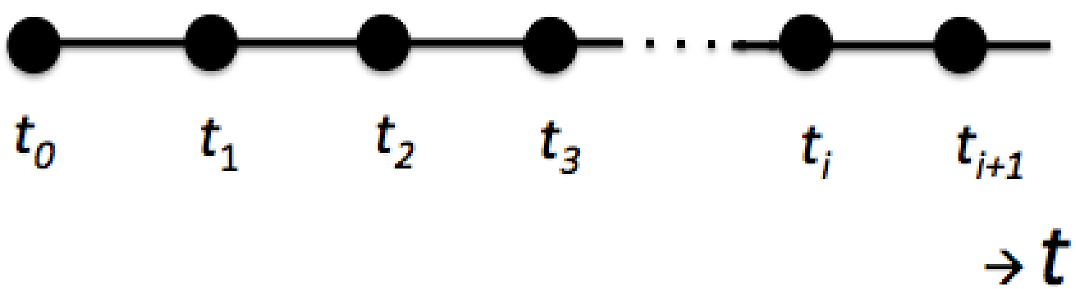
$$\rho_W(x, t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right)$$

Then the probability of finding $W(t)$ in the range $x < W(t) < x + dx$ is given by

$$P\{x \leq W(t) \leq x + dx\} = \rho_W(x, t) dx$$

Connection with diffusion equation: this probability density function is the same as the solution $u(t, x)$ to the diffusion equation if $\alpha = 1/2$, $u(0, x) = \delta(x)$ and $u(t, \pm\infty) = 0$.

NUMERICAL SCHEME



From property 2 of the definition of Brownian motion it directly follows that the difference after a time step Δt is normally distributed with variance Δt:

$$W(t+\Delta t) - W(t) \sim \mathrm{Norm}(0, \Delta t)$$

and hence we can write the following numerical scheme for Brownian motion

$$\boxed{W(t+\Delta t) = W(t) + \sqrt{\Delta t} Z(t)}$$

where $Z(t)$ is a random variable which is normally distributed with variance 1. Note that for every time t we have a *different* random variable $Z(t)$.

Since $kZ(t)$ has a variance of k^2, therefore $\sqrt{\Delta t} Z(t)$ has variance of Δt, thereby obeying property 2 of the Wiener process.

If we start with $W(0) = 0$ we obey property 1 of the Wiener process.

A Wiener process is therefore similar to a random walk with position $W(t)$.

EXAMPLE: SINGLE BROWNIAN WALKER

Example of a random Brownian walk of 4 steps of $W_n = W(t)$ with $t = n\Delta t$ and $\Delta t = 0.1$ and with the random numbers (distributed according to a Gaussian with unit variance and zero mean) $Z_0 = -0.1964$, $Z_1 = -1.01471$, $Z_2 = 0.1479$, and $Z_3 = 1.0803$ is

$$
\begin{aligned}
W_0 &= 0 \\
W_1 &= W_0 + \sqrt{0.1}(-0.1964) = -0.0621 \\
W_2 &= W_1 + \sqrt{0.1}(-1.01471) = -0.3830 \\
W_3 &= W_2 + \sqrt{0.1}(0.1479) = -0.3362 \\
W_4 &= W_3 + \sqrt{0.1}(1.0803) = 0.0054
\end{aligned}
$$

EXAMPLE: SINGLE BROWNIAN WALKER

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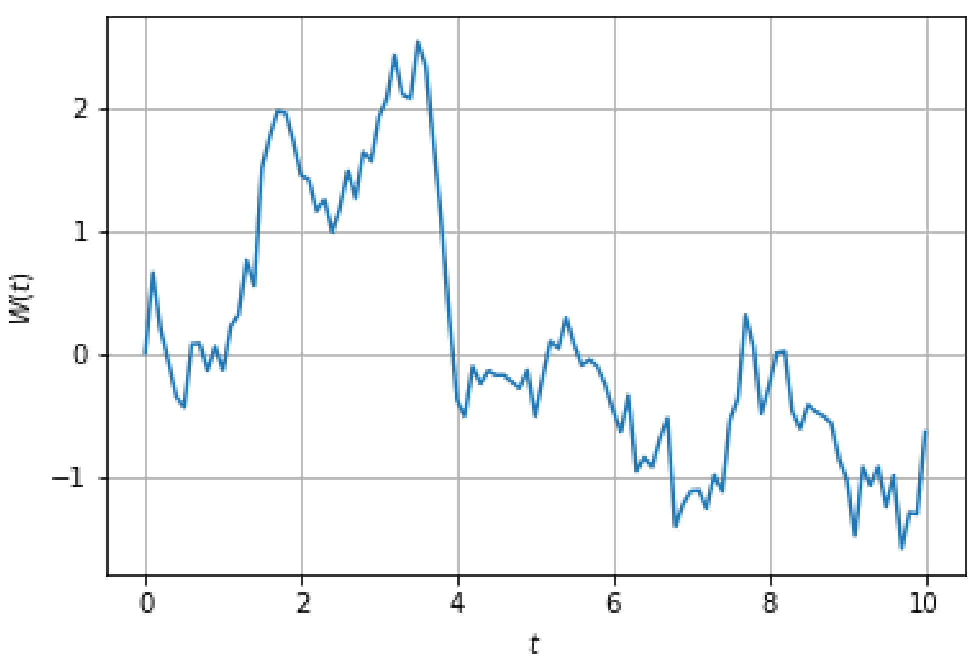
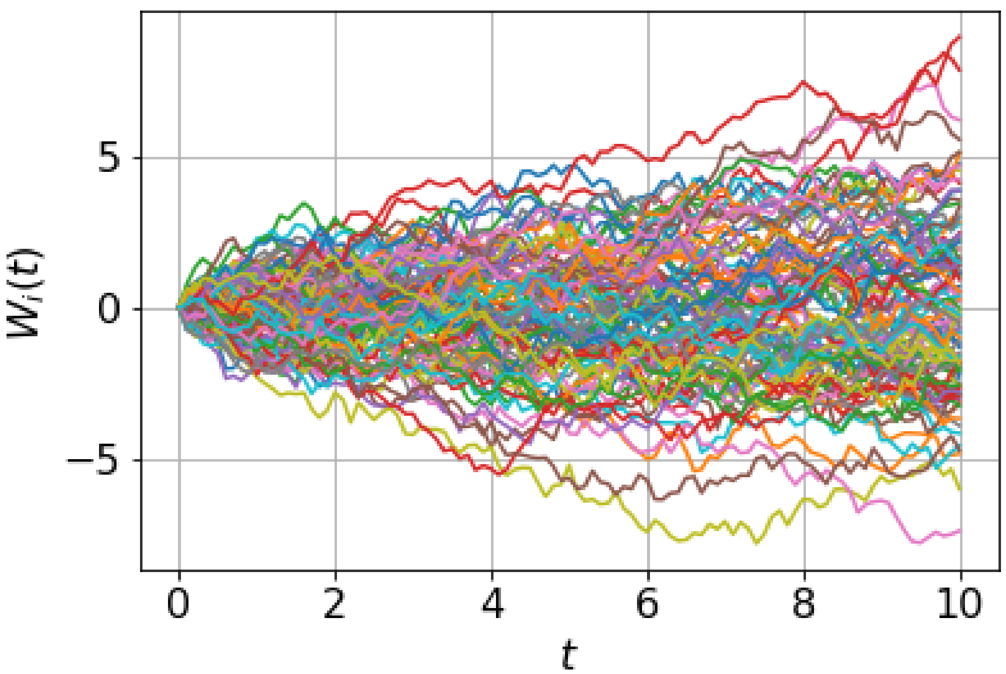


EXAMPLE: 100 BROWNIAN WALKERS

EXAMPLE: 100 BROWNIAN WALKERS



EXAMPLE: HISTOGRAM OF 10,000 BROWNIAN WALKERS AT $t = 10$

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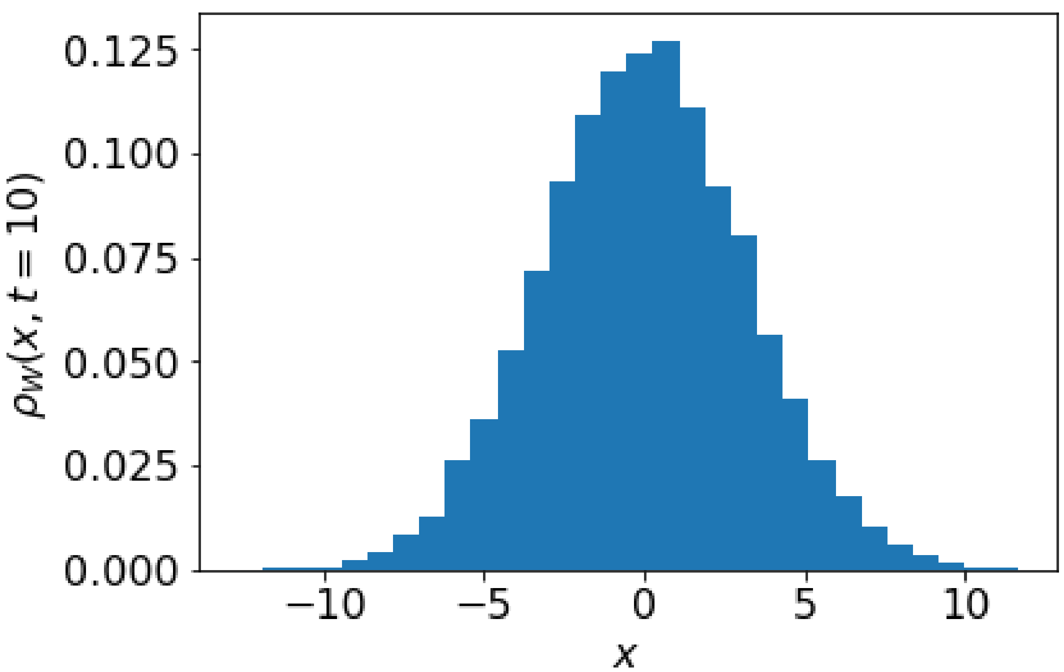
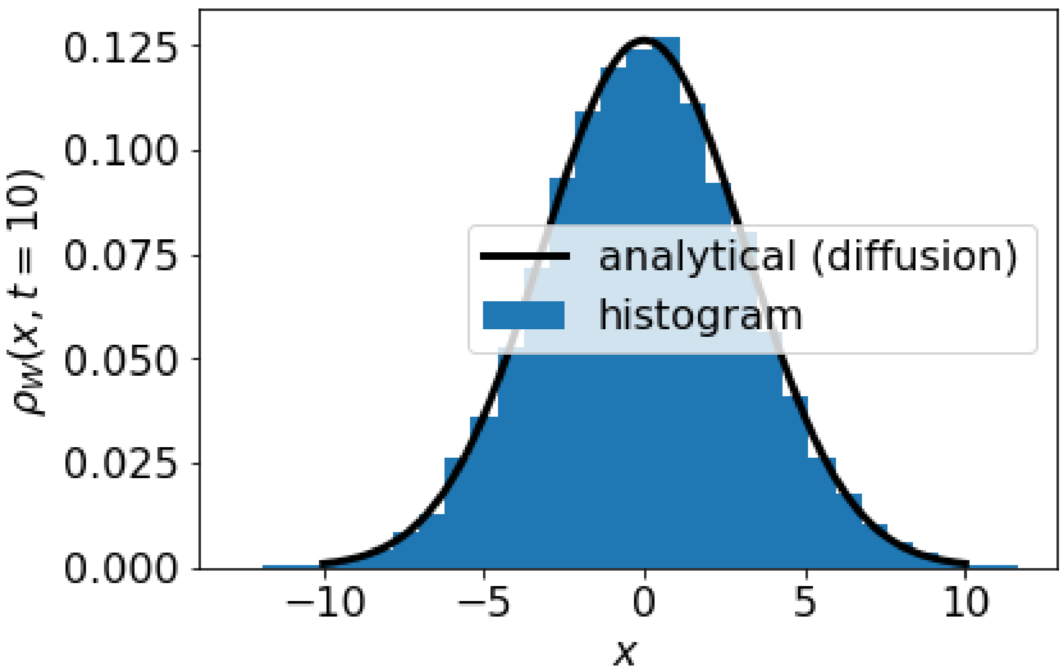
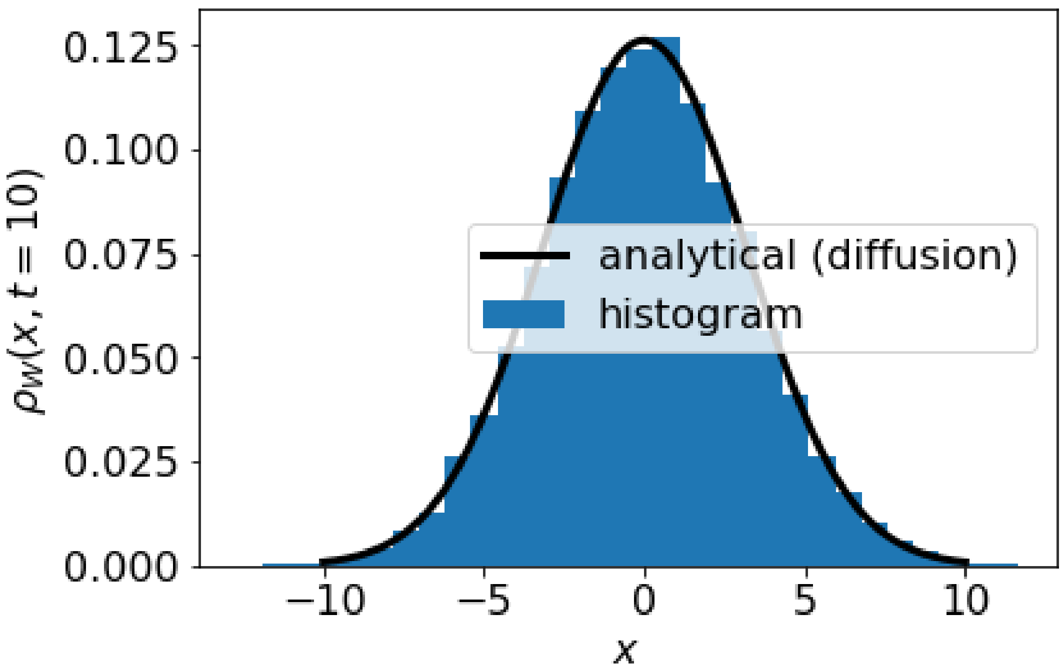



0.125
0.100
0.075
0.050
0.025
0.000
$\rho_W(x, t = 10)$
−10
−5
0
5
10
x
analytical (diffusion)
histogram



A histogram of many Brownian walkers is the same as the solution of the diffusion equation with initial condition the delta function, $u(x, t = 0) = \delta(x)$.

EXTENSIONS

One can extend this description to *geometric Brownian motion* (https://en.wikipedia.org/wiki/Geometric_Brownian_motion), used for (non-negative) stock prices. See also lecture notes of Simon Smith 'Financial mathematics and econo-physics'.

A random walk-approach is also used in Diffusion Monte Carlo (https://en.wikipedia.org/wiki/Diffusion_Monte_Carlo). This is a technique for solving the Schrodinger equation of many electrons in quantum mechanics.

Both are beyond the scope of the current module.

ORNSTEIN-UHLENBECK PROCESS

Another extension is the Ornstein-Uhlenbeck process:

$$dV(t) = dW(t) - kV(t)dt \qquad (*)$$

where $W(t)$ is a Wiener process and k is a positive constant.

Notice that we now have an extra term $-kV(t)dt$ as compared to the Wiener process. It forces the value of $V(t)$ to not deviate too much from zero. If, for example, $V(t)$ is large and positive, then the increment $dV(t)$ will be more likely to be negative.

Note: one may be tempted to write the stochastic differential equation $(*)$ as

$$\frac{dV(t)}{dt} = -kV(t) + \frac{dW(t)}{dt}$$

but the problem is that the Wiener process $W(t)$ is not differentiable in time; it is continuous, but the derivative is not continuous. Hence, strictly speaking, one cannot construct an equation involving derivatives of $W(t)$.

NUMERICAL SCHEME

A numerical scheme for the Ornstein-Uhlenbeck process is

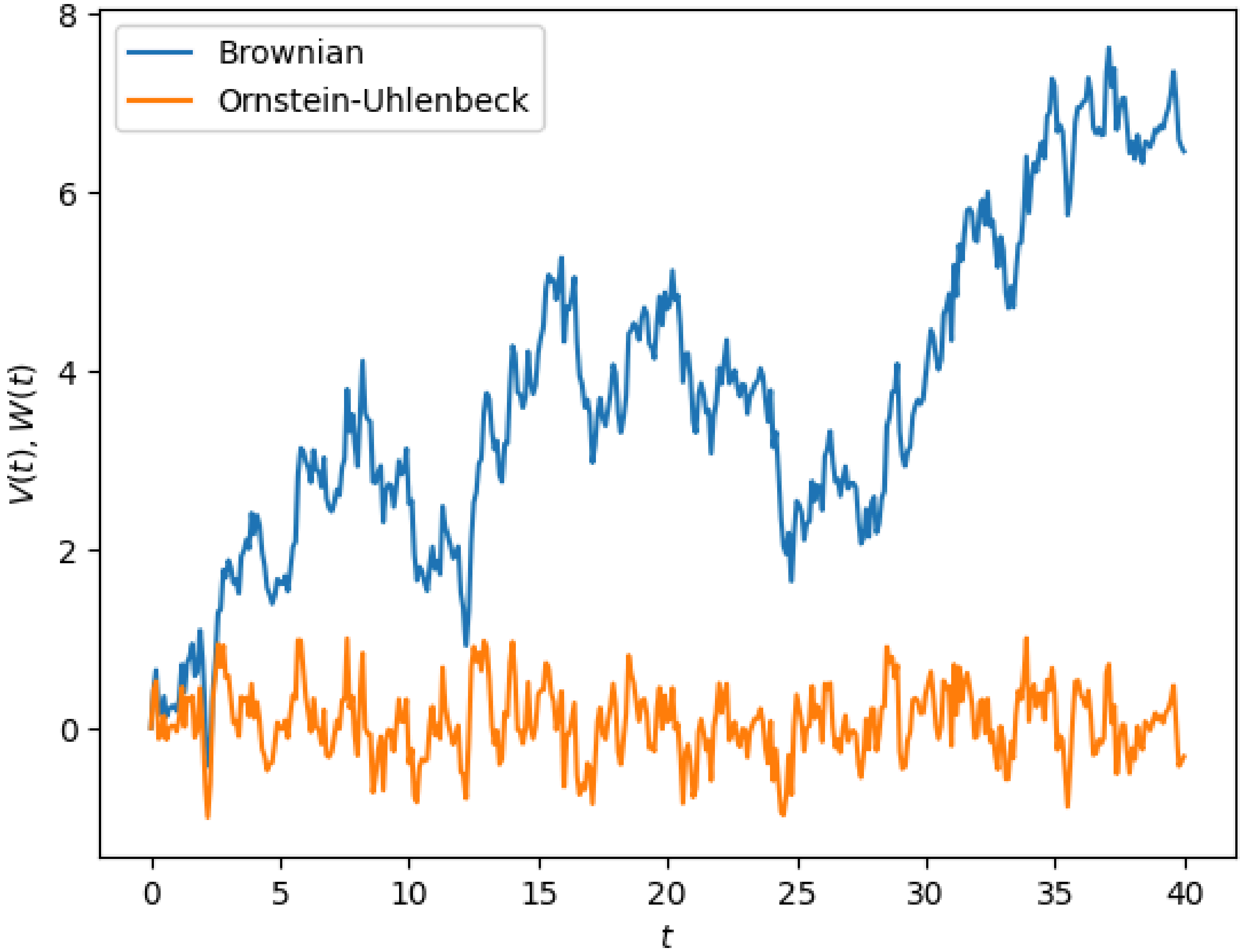
$$V(t+\Delta t) - V(t) = \sqrt{\Delta t} Z(t) - kV(t)\Delta t$$

or, rearranging,

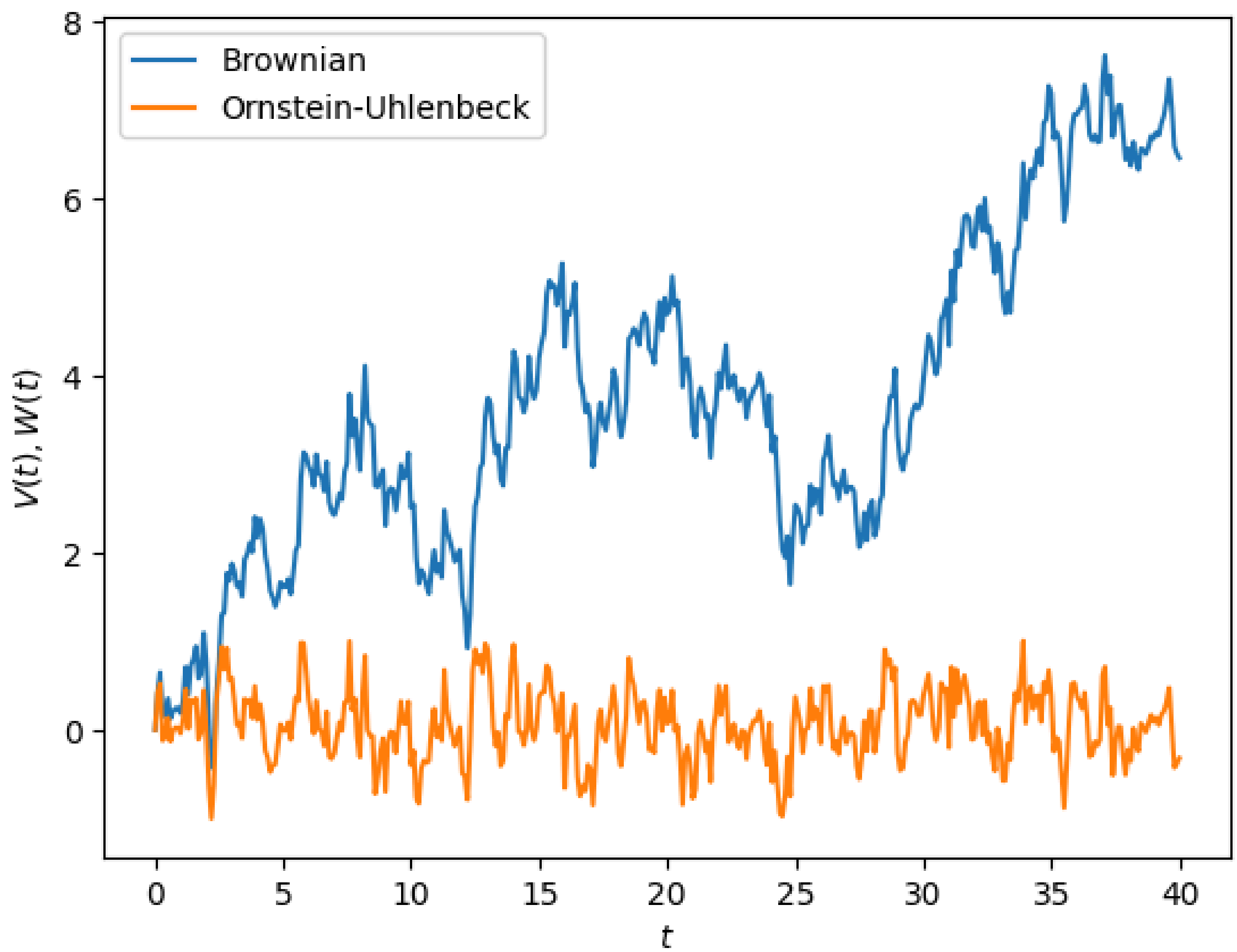
$$\boxed{V(t+\Delta t) = (1-k\Delta t)V(t) + \sqrt{\Delta t} Z(t)}$$

where as with the Wiener process $Z(t)$ is a random variable which is normally distributed with variance 1.

Notice that for $k = 0$ this reduces to the Wiener process.



Brownian
Ornstein-Uhlenbeck
$V(t), W(t)$
t
0
2
4
6
8
0
5
10
15
20
25
30
35
40



Notice that because of the extra term $-kV(t)$ the Ornstein-Uhlenbeck process does not drift away from the origin (as opposed to the Wiener process).

LANGEVIN EQUATION

An alternative description of the Ornstein-Uhlenbeck process

$$dV(t) = -kV(t)dt + dW(t)$$

is by using a **Langevin equation**

$$\frac{dV(t)}{dt} = -kV(t) + \xi(t)$$

where $\xi(t)$ is a delta-correlated fluctuating term, $\langle \xi(t)\xi(t')\rangle = 2\delta(t-t')$. Typically $V(t)$ stands for the velocity of a particle.

The Langevin equation has benefits and drawbacks:

- Benefit: it is more closely related to Newton's law.
- Drawback: one has to be careful for the limit $\Delta t \to 0$, since derivatives are used.

For finite integration steps it can be solved using

$$\frac{V(t+\Delta t) - V(t)}{\Delta t} = -kV(t) + \frac{1}{\sqrt{\Delta t}} Z(t)$$

where $Z(t)$ is again a normally distributed random variable with unit variance. Hence $\xi(t)$ is simply replaced by $Z(t)/\sqrt{\Delta t}$.

A more general Langevin equation is

$$m\frac{d^2X(t)}{dt^2} = -\zeta V(t) + F(X(t)) + \xi(t)$$

This models a particle with position $X(t)$ under the influence of a random force due to kicks $\xi(t)$ and a regular force $F(X)$ at position X, which may be caused by a potential $-dU(x)/dx$.

EXERCISES SESSION 8

1. What is the difference between a Wiener process and an Ornstein-Uhlenbeck process? In which limit would they be equal to each other?

2. How to numerically implement the Dirac delta function as an initial condition in solving a PDE?

3. For the remaining exercises, see the Assessment section on Blackboard.