Notes on probability distributions and their interpretation

Contents

I. DISCRETISATION AND PROBABILITIES

A. Discretisation of the one-particle Schrödinger equation

To help reasoning about probabilities it is convenient to think about discretisations of the Schrödinger equation. We consider a one-dimensional one-particle system with Schrödinger equation:

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + v(x)\right)\varphi(x) = \epsilon\varphi(x) \tag{1}$$

where x is a one-dimensional real coordinate and where we impose the boundary condition $\varphi(0) = \varphi(L) = 0$. We can write this as

$$(\hat{H}\varphi)(x) = \epsilon\varphi(x) \tag{2}$$

where $\hat{H} = \hat{T} + \hat{V}$ is the Hamilton operator and where the kinetic and potential energy operator are defined as:

$$(\hat{T}\varphi)(x) = -\frac{1}{2}\frac{d^2\varphi}{dx^2} \qquad (\hat{V}\varphi)(x) = v(x)\varphi(x) \tag{3}$$

Suppose we want to solve this problem on a computer, then we need to find a numerical procedure to solve the differential equation. An obvious approach is to use discretisation where we evaluate φ in a discrete number n of points x_i for which we would like to evaluate the values $\varphi_i = \varphi(x_i)$. We take

$$x_i = i\,\Delta L \qquad \Delta L = \frac{L}{n+1} \tag{4}$$

such that $x_0 = 0$ and $x_{n+1} = L$ such that with our boundary conditions $\varphi(x_0) = 0$ and $\varphi(x_{n+1}) = 0$. We now want to evaluate $\varphi(x)$ in the n remaining points $(x_1, \ldots, x_n)$. We denote by φ the n-dimenional vector:

$$\varphi = (\varphi(x_1), \ldots, \varphi(x_n)) = (\varphi_1, \ldots, \varphi_n) \tag{5}$$

The action of the operator $\hat{V}$ in Eq.(88) is simply

$$(\hat{V}\varphi)(x_i) = v(x_i)\varphi(x_i) \tag{6}$$

In our discretised version this simply maps the vector $\varphi = (\varphi_1, \ldots, \varphi_n)$ to

$$(V\varphi) = (v_1\varphi_1, \ldots, v_n\varphi_n) = \begin{pmatrix} v_1 & 0 & \ldots & \ldots & 0 \\ 0 & v_2 & 0 & \ldots & \vdots \\ \vdots & 0 & \ddots & \ldots & \vdots \\ \vdots & & & v_{n-1} & 0 \\ 0 & \ldots & \ldots & 0 & v_n \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \vdots \\ \varphi_n \end{pmatrix} \tag{7}$$

where we defined the diagonal matrix V by

$$V = \begin{pmatrix} v_1 & 0 & \dots & \dots & 0 \\ 0 & v_2 & 0 & \dots & \vdots \\ \vdots & 0 & \ddots & \dots & \vdots \\ \vdots & & & v_{n-1} & 0 \\ 0 & \dots & \dots & 0 & v_n \end{pmatrix} \tag{8}$$

So the potential operator acting on the discretised version of the wavefunction φ is simply represented by the diagonal matrix V. We now want to derive a matrix representation of the kinetic energy operator $\hat{T}$. To do this we consider the following to Taylor series

$$\varphi(x_{i+1}) = \varphi(x_i + \Delta L) = \varphi(x_i) + \Delta L \frac{d\varphi}{dx}(x_i) + \frac{(\Delta L)^2}{2}\frac{d^2\varphi}{dx^2}(x_i) + \dots \tag{9}$$

$$\varphi(x_{i-1}) = \varphi(x_i - \Delta L) = \varphi(x_i) - \Delta L \frac{d\varphi}{dx}(x_i) + \frac{(\Delta L)^2}{2}\frac{d^2\varphi}{dx^2}(x_i) + \dots \tag{10}$$

Adding both expansions and neglecting higher order terms than $(\Delta L)^2$ give the equation

$$\varphi(x_{i-1}) + \varphi(x_{i+1}) = 2\varphi(x_i) + (\Delta L)^2 \frac{d^2\varphi}{dx^2}(x_i) \tag{11}$$

and we thus obtain

$$\frac{d^2\varphi}{dx^2}(x_i) = \frac{1}{(\Delta L)^2}(\varphi(x_{i-1}) - 2\varphi(x_i) + \varphi(x_{i+1})) \tag{12}$$

an equation which becomes more accurate when $n \to \infty$ and $\Delta L = L/(n+1) \to 0$ (in fact you can check from the Taylor expansion that the error is of order $(\Delta L)^2$ since odd powers cancel in the addition we used above). Taking into account the boundary conditions $\varphi(x_0) = \varphi(x_{n+1}) = 0$ we see that we can write Eq.(12) as

$$\begin{pmatrix} \frac{d^2\varphi}{dx^2}(x_1) \\ \vdots \\ \vdots \\ \frac{d^2\varphi}{dx^2}(x_n) \end{pmatrix} = \frac{1}{(\Delta L)^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{n-1} \\ \varphi_n \end{pmatrix} \tag{13}$$

and therefore we can represented the kinetic energy operator as

$$\begin{pmatrix} (\hat{T}\varphi)(x_1) \\ \vdots \\ \vdots \\ (\hat{T}\varphi)(x_n) \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \frac{d^2\varphi}{dx^2}(x_1) \\ \vdots \\ \vdots \\ \frac{d^2\varphi}{dx^2}(x_n) \end{pmatrix} = -\frac{1}{2(\Delta L)^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{n-1} \\ \varphi_n \end{pmatrix} = T\varphi \tag{14}$$

where we defined the matrix

$$T = -\frac{1}{2(\Delta L)^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix} \tag{15}$$

We this find that the Hamiltonian of our system can be described by the matrix

$$H = T + V = -\frac{1}{2(\Delta L)^2}\begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & & \ddots & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix} + \begin{pmatrix} v_1 & 0 & \dots & \dots & 0 \\ 0 & v_2 & 0 & \dots & \vdots \\ \vdots & 0 & \ddots & \dots & \vdots \\ \vdots & & & v_{n-1} & 0 \\ 0 & \dots & \dots & 0 & v_n \end{pmatrix} \tag{16}$$

Diagonalising this matrix then gives the desired eigenvectors φ and their eigenenergies. We can also give a formula for the matrix elements of this matrix in terms of Kronecker delta functions:

$$H_{ij} = -\frac{1}{2(\Delta L)^2}(\delta_{i,j+1} - 2\,\delta_{ij} + \delta_{i,j-1}) + v_i\delta_{ij} \tag{17}$$

where $i, j \in \{1, \dots, n\}$. We can readily check that indeed

$$\sum_{j=1}^{n} H_{ij}\varphi_j = -\frac{1}{2(\Delta L)^2}(\varphi_{i-1} - 2\varphi_i + \varphi_{i+1}) + v_i\varphi_i \tag{18}$$

as desired, so that the Schrödinger equation is transformed into the matrix equation

$$\sum_{j=1}^{n} H_{ij}\varphi_j = \epsilon\varphi_i \tag{19}$$

Since the Hamilton matrix H is real we can choose the corresponding eigenfunctions to be real as well. We also have to choose a normalisation of the eigenfunctions. ' If we replace the norm integral of the continuum case by a Riemann sum we have

$$1 = \int_0^L dx\,\varphi^2(x) \approx \Delta L \sum_{i=1}^{n} \varphi(x_i)^2 \tag{20}$$

and therefore we require the vector φ to be normalised according to

$$\sum_{i=1}^{n} \varphi_i^2 = \frac{1}{\Delta L} \tag{21}$$

We can thus always write

$$(\varphi_1, \dots, \varphi_n) = \frac{1}{\sqrt{\Delta L}}(\psi_1, \dots, \psi_n) \tag{22}$$

where

$$\sum_{j=1}^{n} H_{ij}\psi_j = \epsilon\psi_i \qquad \sum_{i=1}^{n} \psi_i^2 = 1 \tag{23}$$

which is a useful expression since practical diagonalisation routines use this normalisation. As an example we solve numerically the harmonic oscillator

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2(x - \frac{L}{2})^2\right)\varphi(x) = \epsilon\varphi(x) \tag{24}$$

on the interval $[0, L]$ for $L = 1$. We choose $\omega = 100$ so that the wavefunctions fit nicely in the interval and we take $n = 400$. The result and the comparison to the analytic normalised solution

$$\psi_m(x) = \frac{1}{\sqrt{2^m m!}}(\frac{\omega}{\pi})^{\frac{1}{4}} e^{-\frac{\omega}{2}(x-\frac{L}{2})^2} H_m(\sqrt{\omega}(x - \frac{L}{2})) \tag{25}$$

for the m-th excited state (where H_m is the m-th Hermite polynomial) is given in the short Mathematica code attached to the end of these notes. You can play around with this code to solve the Schrödinger equation for other potentials.

B. A finite Hilbert space perspective: one particle

For the generalisation to more particles and for getting a deeper insight in general it is useful to view the expansion in the previous section from the viewpoint of a basis set expansion. For the points $x_i = i\Delta L$ with $i \in \{1, \dots, n\}$ and $\Delta L = L/(n+1)$ we let

$$\mathcal{I}_i = [\, x_i - \frac{\Delta L}{2}, x_i + \frac{\Delta L}{2}\,[= [\,(i - \frac{1}{2})\Delta L, (i + \frac{1}{2})\Delta L\,[\tag{26}$$

be an half-open interval of length ΔL centred around x_i (where we remind that $x \in [a, b[$ means $a \leq x < b$). We define the normalised functions

$$e_i(x) = \begin{cases} \frac{1}{\sqrt{\Delta L}} & x \in \mathcal{I}_i \\ 0 & x \notin \mathcal{I}_i \end{cases} \tag{27}$$

so that $e_i(x)$ represents a state in which there is a particle in interval $\mathcal{I}_i$ with certainty. The functions $e_i(x)$ have the properties

$$e_i(x)e_j(x) = \delta_{ij}e_i^2(x) \qquad \int_0^L dx\, e_i(x)^* e_j(x) = \delta_{ij} \tag{28}$$

and so the functions $e_i(x)$ for $i \in \{1, \ldots, n\}$ form an n-dimensional orthonormal basis. We now consider the n-dimensional complex Hilbert space $\mathcal{H}_n$ spanned by the functions $e_i(x)$. An arbitrary function in $\mathcal{H}_n$ is thus of the form

$$\Psi(x) = \sum_{i=1}^{n} \psi_i\, e_i(x) \tag{29}$$

for some coefficients ψ_i. If Ψ is normalised then we have

$$1 = \langle \Psi | \Psi \rangle = \sum_{i,j=1}^{n} \psi_i^* \psi_j \langle e_i | e_j \rangle = \sum_{i=1}^{n} |\psi_i|^2 \tag{30}$$

We thus see that we can interpret the coefficients ψ_i in Eq.(29) as probability amplitudes. Since $e_i(x)$ described a state in which there is a particle in interval $\mathcal{I}_i$ with certainty we see that:

$$|\psi_i|^2 = \text{ the probability that the particle is located in interval } \mathcal{I}_i \tag{31}$$

If we want $\Psi(x)$ to approximate a continuum solution for a single particle in a potential $v(x)$ then we can take ψ_i to satisfy Eq.(23) for the Hamilton matrix with the matrix elements of Eq.(17). If we take always real eigenvectors, then in every point x_j the function $\Psi(x)$ agrees with $\varphi(x_j)$ of the previous section since

$$\Psi(x_j) = \sum_{i=1}^{n} \psi_i\, e_i(x_j) = \sum_{i=1}^{n} \psi_i \frac{\delta_{ij}}{\sqrt{\Delta L}} = \frac{\psi_j}{\sqrt{\Delta L}} = \varphi_j \tag{32}$$

where we used Eq.(22). From Eq.(31) we thus see that

$$|\Psi(x_j)|^2\, \Delta L = |\psi_i|^2 = \text{ the probability that the particle is located in interval } \mathcal{I}_i \tag{33}$$

In the limit $n \to \infty$ or $\Delta L = L/(n+1) \to 0$ the function $\Psi(x)$ then converges to the normalised continuum solution $\varphi(x)$ of Eq.(24).

C. A finite Hilbert space perspective: many particles

Now we turn our attention to the case of N fermionic particles in one spatial dimension, where all particles are located in the interval $[0, L]$. For simplicity we neglect spin so we are dealing with so-called spinless fermions which are described by purely spatial anti-symmetric wavefunctions. We start by defining the Slater determinants out of the one-particle functions $e_i(x)$, i.e. we define:

$$e_I(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} e_{i_1}(x_1) & \ldots & e_{i_N}(x_1) \\ \vdots & & \vdots \\ e_{i_1}(x_N) & \ldots & e_{i_N}(x_N) \end{vmatrix} = \frac{1}{\sqrt{N!}} \sum_{\sigma} (-1)^{|\sigma|} e_{\sigma(i_1)}(x_1) \ldots e_{\sigma(i_N)}(x_N) \tag{34}$$

where $I = (i_1, \ldots, i_N)$ is a multi-index in which $i_1 < \ldots < i_N$ and $i_k \in \{1, \ldots, n\}$, which also implies that $n \geq N$. In the last step σ denotes a permutation of N elements and $|\sigma|$ denotes its parity, while the sum extends over all $N!$ permutations. Note that here the variables x_j denote continuum spatial variables for particle j and not grid points. The states e_I form an orthonormal set:

$$\langle e_I | e_J \rangle = \int_0^L dx_1 \ldots d_N e_I(x_1, \ldots, x_N)^* e_J(x_1, \ldots, x_N) = \delta_{IJ} = \delta_{i_1 j_1} \ldots \delta_{i_N j_N} \tag{35}$$

where $J = (j_1, \dots, j_N)$ with $j_1 < \dots < j_N$. The function e_I describes a state in which there is a particle in the intervals $\mathcal{I}_{i_1}, \dots, \mathcal{I}_{i_N}$ with certainty. A general N-particle state Ψ can then be expanded in these state

$$\Psi(x_1, \dots, x_N) = \sum_I \Psi_I \, e_I(x_1, \dots, x_N) \tag{36}$$

where the sum is over all ordered multi-indices $I = (i_1, \dots, i_N)$ with $i_1 < \dots < i_N$ and $i_k \in \{1, \dots, n\}$. If we take Ψ to be normalised we have

$$1 = \langle \Psi | \Psi \rangle = \sum_{I,J} \Psi_I^* \Psi_J \langle e_I | e_J \rangle = \sum_{I,J} \Psi_I^* \Psi_J \delta_{IJ} = \sum_I |\Psi_I|^2 \tag{37}$$

In view of the probability interpretation of e_I, we can assign to Ψ_I the following meaning:

$$|\Psi_I|^2 = \text{ the probability to find a particle in all of the intervals } \mathcal{I}_{i_1}, \dots, \mathcal{I}_{i_N} \tag{38}$$

Let is now select N coordinates $x_k \in \mathcal{I}_{j_k}$ with $j_1 < \dots < j_N$. Then

$$\Psi(x_1, \dots, x_N) = \sum_I \Psi_I \, e_I(x_1, \dots, x_N) = \sum_I \Psi_I \, \frac{1}{\sqrt{N!}} \frac{1}{(\sqrt{\Delta L})^N} \delta_{i_1 j_1} \dots \delta_{i_N j_N} = \frac{\Psi_J}{\sqrt{N!}(\sqrt{\Delta L})^N} \tag{39}$$

So we also find that for $x_k \in \mathcal{I}_{i_k}$ we have

$$N! |\Psi(x_1, \dots, x_N)|^2 (\Delta L)^N = |\Psi_I|^2 = \text{ the probability to find a particle in all of the intervals } \mathcal{I}_{i_1}, \dots, \mathcal{I}_{i_N} \tag{40}$$

In the next step we are going to look at the particle density $n(x)$ and the pair density $\Gamma(x, x')$. To do that it is actually more instructive to look at these quantities from a more general point of view. We define the diagonal k-particle density matrix as

$$\Gamma_k(x_1, \dots, x_k) = \frac{N!}{(N-k)!} \int dx_{k+1} \dots dx_N |\Psi(x_1, \dots, x_N)|^2 \tag{41}$$

Then $\Gamma_N = N! |\Psi|^2$ and Eq.(40), for $x_k \in \mathcal{I}_{i_k}$, becomes

$$\Gamma_N(x_1, \dots, x_N)|^2 (\Delta L)^N = |\Psi_I|^2 = \text{ the probability to find a particle in all of the intervals } \mathcal{I}_{i_1}, \dots, \mathcal{I}_{i_N} \tag{42}$$

The density is then given by $n(x) = \Gamma_1(x)$ and the pair-density by $\Gamma(x, x') = \Gamma_2(x, x')$. Since Ψ is normalised the diagonal density matrix satisfies

$$\int dx_1 \dots dx_k \, \Gamma_k(x_1, \dots, x_k) = \frac{N!}{(N-k)!} \tag{43}$$

so that, in particular:

$$\int dx \, n(x) = N \qquad\qquad \int dx dx' \, \Gamma(x, x') = N(N-1) \tag{44}$$

Another useful relation is

$$\begin{aligned} \int dx_k \, \Gamma_k(x_1, \dots, x_k) &= \frac{N!}{(N-k)!} \int dx_k \dots dx_N |\Psi(x_1, \dots, x_N)|^2 \\ &= \frac{N!}{(N-k)!} \frac{(N-(k-1))!}{N!} \Gamma_{k-1}(x_1, \dots, x_{k-1}) = (N-k+1) \Gamma_{k-1}(x_1, \dots, x_{k-1}) \end{aligned} \tag{45}$$

Let us now calculate Γ_k for an arbitrary state of the form of Eq.(36) in our finite Hilbert space. Before doing that let us first derive an equation that we will use in that calculation. We have

$$\begin{aligned} e_I(x_1, \dots, x_N)^* e_J(x_1, \dots, x_N) &= \frac{1}{N!} \sum_{\sigma, \pi} (-1)^{|\sigma| + |\pi|} e_{\sigma(i_1)}(x_1) \dots e_{\sigma(i_N)}(x_N) e_{\pi(i_1)}(x_1) \dots e_{\pi(i_N)}(x_N) \\ &= \frac{1}{N!} \sum_{\sigma, \pi} (-1)^{|\sigma| + |\pi|} (-1)^{|\sigma| + |\pi|} \delta_{\sigma(i_1)\pi(j_1)} \dots \delta_{\sigma(i_N)\pi(j_N)} e^2_{\sigma(i_1)}(x_1) \dots e^2_{\sigma(i_N)}(x_N) \end{aligned} \tag{46}$$

where we used the first property in Eq.(28) and σ and π denote permutations of N elements. We see that if I and J are not the same sets then at least one of the Kronecker delta functions must vanish and therefore we have only a nonzero result when $I = J$. In that case we also must have that $\pi = \sigma$ to avoid zero terms and we thus obtain

$$e_I(x_1, \dots, x_N)^* e_J(x_1, \dots, x_N) = \frac{\delta_{IJ}}{N!} \sum_\sigma e^2_{\sigma(i_1)}(x_1) \dots e^2_{\sigma(i_N)}(x_N) \tag{47}$$

If we use this expression then we can readily calculate the diagonal k-particle density matrix to be:

$$\begin{aligned}
\Gamma_k(x_1, \dots, x_k) &= \sum_{I,J} \Psi^*_I \Psi_J \frac{N!}{(N-k)!} \int dx_{k+1} \dots dx_N e_I(x_1, \dots, x_N)^* e_J(x_1, \dots, x_N) \\
&= \frac{1}{(N-k)!} \sum_{I,J} \Psi^*_I \Psi_J \delta_{IJ} \sum_\sigma \int dx_{k+1} \dots dx_N e^2_{\sigma(i_1)}(x_1) \dots e^2_{\sigma(i_N)}(x_N) \\
&= \frac{1}{(N-k)!} \sum_I |\Psi_I|^2 \sum_\sigma e^2_{\sigma(i_1)}(x_1) \dots e^2_{\sigma(i_k)}(x_k)
\end{aligned} \tag{48}$$

We can write this as

$$\Gamma_k(x_1, \dots, x_k) = \sum_{j_1, \dots, j_k = 1}^{n} \Gamma_{j_1 \dots j_k} e^2_{j_1}(x_1) \dots e^2_{j_k}(x_k) \tag{49}$$

where we defined

$$\Gamma_{j_1 \dots j_k} = \frac{1}{(N-k)!} \sum_I |\Psi_I|^2 \sum_\sigma \delta_{j_1 \sigma(i_1)} \dots \delta_{j_k \sigma(i_k)} \tag{50}$$

This expression also implies that

$$\Gamma_{j_1 \dots j_k} = \Gamma_{\tau(j_1) \dots \tau(j_k)} \tag{51}$$

for any permutation τ of k elements. Now for any permutation of N elements there are $(N-k)!$ permutations that map $(i_1, \dots, i_k)$ to $(j_1, \dots, j_k)$ and this only gives a nonzero contribution when the elements $\{j_1, \dots, j_k\}$ are contained in the multi-index I, typically in a reordered fashion, which we denote by $I \ni \{j_1, \dots, j_k\}$. So it therefore follows that

$$\Gamma_{j_1 \dots j_k} = \sum_{I \ni \{j_1, \dots, j_k\}} |\Psi_I|^2 \tag{52}$$

where we sum over all ordered multi-indices I containing the integers $\{j_1, \dots, j_k\}$. Note that the set $\{j_1, \dots, j_k\}$ is not necessarily ordered and that the labels typically occur in a reordered fashion in the multi-index I. Clearly from Eq.(52) it follows that $\Gamma_{j_1 \dots j_k}$ is zero when the labels $\{j_1, \dots, j_k\}$ are not distinct. From the probability interpretation in Eq.(53) it then follows

$$\Gamma_{j_1 \dots j_k} = \text{ the probability to find a particle in all of the intervals } \mathcal{I}_{i_1}, \dots, \mathcal{I}_{i_k} \tag{53}$$

Further, choosing $x_l \in \mathcal{I}_{i_l}$ gives

$$\Gamma_k(x_1, \dots, x_k) = \sum_{j_1, \dots, j_k = 1}^{n} \Gamma_{j_1 \dots j_k} e^2_{j_1}(x_1) \dots e^2_{j_k}(x_k) = \sum_{j_1, \dots, j_k = 1}^{n} \Gamma_{j_1 \dots j_k} \frac{1}{(\Delta L)^k} \delta_{i_1 j_1} \dots \delta_{i_k j_k} = \frac{\Gamma_{i_1 \dots i_k}}{(\Delta L)^k} \tag{54}$$

such that Eq.(53) implies that, for $x_l \in \mathcal{I}_{i_l}$:

$$\Gamma_k(x_1, \dots, x_k)(\Delta L)^k = \Gamma_{j_1 \dots j_k} = \text{ the probability to find a particle in all of the intervals } \mathcal{I}_{i_1}, \dots, \mathcal{I}_{i_k} \tag{55}$$

which clearly illustrates the physical meaning of the diagonal k-particle density matrix. We continue by deriving a few useful relations. We have

$$\Gamma_{j_1 \dots j_k} = \sum_{I \ni \{j_1, \dots, j_k\}} |\Psi_I|^2 \leq \sum_I |\Psi_I|^2 = 1 \tag{56}$$

and therefore

$$0 \leq \Gamma_{j_1 \ldots j_k} \leq 1 \tag{57}$$

The expression (52) also implies that

$$\Gamma_{j_1 \ldots j_k} = \sum_{I \ni \{j_1, \ldots, j_k\}} |\Psi_I|^2 \leq \sum_{I \ni \{j_1, \ldots, j_{k-1}\}} |\Psi_I|^2 = \Gamma_{j_1 \ldots j_{k-1}} \tag{58}$$

From Eq.(43) it follows further that

$$\frac{N!}{(N-k)!} = \sum_{j_1, \ldots, j_k = 1}^{n} \Gamma_{j_1 \ldots j_k} \int dx_1 \ldots dx_k e^2_{j_1}(x_1) \ldots e^2_{j_N}(x_N) = \sum_{j_1, \ldots, j_k = 1}^{n} \Gamma_{j_1 \ldots j_k} \tag{59}$$

while Eq.(45) tells us that

$$\sum_{j_k=1}^{n} \Gamma_{j_1 \ldots j_k} = (N - k + 1)\, \Gamma_{j_1 \ldots j_{k-1}} \tag{60}$$

The probabilities in Eq.(59) do not add up to one because the probability events we consider are not exclusive; we will address this issue in detail below. In particular for the density, $n = \Gamma_1$, we have the relations

$$n(x) = \sum_{i=1}^{n} n_i\, e_i^2(x) \qquad\qquad n_i = \sum_{I \ni i} |\Psi_I|^2 \qquad\qquad \sum_{i=1}^{n} n_i = N \tag{61}$$

Let $y_j \in \mathcal{I}_j$ be a coordinates in interval $\mathcal{I}_j$, then we see that

$$n(y_j) = \sum_{i=1}^{n} n_i\, e_i^2(y_j) = \sum_{i=1}^{n} n_i\, \frac{\delta_{ij}}{\Delta L} = \frac{n_j}{\Delta L} \tag{62}$$

We therefore see that

$$n(y_j) \Delta L = n_j = \text{ the probability to find a particle in the interval } \mathcal{I}_j \tag{63}$$

which therefore assigns a clear probability interpretation to the density (and which is a special case of Eq.(55) for $k = 1$). We can derive analogous formulas for the pair density $\Gamma = \Gamma_2$:

$$\Gamma(x, x') = \sum_{i,j=1}^{n} \Gamma_{ij}\, e_i^2(x) e_j^2(x') \qquad\qquad \Gamma_{ij} = \sum_{I \ni \{i,j\}} |\Psi_I|^2 \qquad\qquad \sum_{i,j=1}^{n} \Gamma_{ij} = N(N-1) \tag{64}$$

while Eqs.(58) and (60) imply that

$$\Gamma_{ji} = \Gamma_{ij} \leq n_i \qquad\qquad \sum_{j=1}^{n} \Gamma_{ij} = (N-1) n_i \tag{65}$$

Let y_k and y_l be coordinates in the intervals $\mathcal{I}_k$ and $\mathcal{I}_l$, then we see that

$$\Gamma(y_k, y_l) = \sum_{i,j=1}^{n} \Gamma_{ij}\, e_i^2(y_k) e_j^2(y_l) = \sum_{i,j=1}^{n} \Gamma_{ij}\, \frac{\delta_{ik}\delta_{jl}}{(\Delta L)^2} = \frac{\Gamma_{kl}}{(\Delta L)^2} \tag{66}$$

We therefore see that

$$\Gamma(y_k, y_l)(\Delta L)^2 = \Gamma_{kl} = \text{ the probability to find a particle in the interval } \mathcal{I}_k \text{ and another one in interval } \mathcal{I}_l \tag{67}$$

which again is a special case of Eq.(55) for $k = 2$. We can continue calculating conditional probabilities. We have

$$p(i|j) = \frac{\Gamma_{ij}}{n_j} = \text{ the probability to find a particle in the interval } \mathcal{I}_i \text{ given that we know that there is a particle in interval } \mathcal{I}_j \tag{68}$$

where the first expression in Eq.(65) tells us that $0 \leq p(i|j) \leq 1$ as it should. From the equations above we see that for $y_i \in \mathcal{I}_i$ and $y_j \in \mathcal{I}_j$

$$p(i|j) = \frac{\Gamma_{ij}}{n_j} = \frac{\Gamma(y_i, y_j)(\Delta L)^2}{n(y_j)\Delta L} = \frac{\Gamma(y_i, y_j)}{n(y_j)}\Delta L \tag{69}$$

and from Eq.(65) we see that

$$\sum_{i=1}^{n} p(i|j) = \frac{1}{n_j}\sum_{i=1}^{n}\Gamma_{ij} = N - 1 \tag{70}$$

Again the probabilities do not sum to one in general, since the conditional probability to find a particle in interval $\mathcal{I}_i$ do not exclude the possibility of there being another particle in another interval, unless $N = 2$ in which case the sum of the probabilities is indeed equal to one.

D. An illustrative example

We illustrate the basic probability concepts with a very basic example of three particles and four intervals, we have $N = 3$ and $n = 4$. Then a general 3-particle state is of the form

$$\Psi = \Psi_{123}\, e_{123} + \Psi_{124}\, e_{124} + \Psi_{134}\, e_{134} + \Psi_{234}\, e_{234} \tag{71}$$

where for compact notation we do no write the arguments of Ψ and the functions $e_{i_1 i_2 i_3}$. Since the function is normalised we have

$$1 = |\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{134}|^2 + |\Psi_{234}|^2 \tag{72}$$

The density coefficients n_i are readily calculated from the second expression in Eq.(61) to be

$$n_1 = |\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{134}|^2 \tag{73}$$
$$n_2 = |\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{234}|^2 \tag{74}$$
$$n_3 = |\Psi_{123}|^2 + |\Psi_{134}|^2 + |\Psi_{234}|^2 \tag{75}$$
$$n_4 = |\Psi_{124}|^2 + |\Psi_{134}|^2 + |\Psi_{234}|^2 \tag{76}$$

Summing the densities we find

$$n_1 + n_2 + n_3 + n_4 = 3(|\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{134}|^2 + |\Psi_{234}|^2) = 3 \tag{77}$$

so the density indeed sums up to three. The reason that the densities do not sum to one is that the finding a particle in interval $\mathcal{I}_i$ does not exclude that we can find another particle in another interval $\mathcal{I}_j$, so these probabilities are not exclusive. This is clear since for any index $i \in I$ in our example there are two indices referring to particles in other intervals. Only for a one-particle system this is not the case and indeed in that case the density coefficients n_i sum up to $N = 1$. For the pair densities we have from the second expression in Eq.(64):

$$\Gamma_{12} = |\Psi_{123}|^2 + |\Psi_{124}|^2 \qquad \Gamma_{23} = |\Psi_{123}|^2 + |\Psi_{234}|^2 \tag{78}$$
$$\Gamma_{13} = |\Psi_{123}|^2 + |\Psi_{134}|^2 \qquad \Gamma_{24} = |\Psi_{124}|^2 + |\Psi_{234}|^2 \tag{79}$$
$$\Gamma_{14} = |\Psi_{124}|^2 + |\Psi_{134}|^2 \qquad \Gamma_{34} = |\Psi_{134}|^2 + |\Psi_{234}|^2 \tag{80}$$

and $\Gamma_{ji} = \Gamma_{ij}$. From this we can confirm the last expression in Eq.(64):

$$\sum_{ij}\Gamma_{ij} = 2\sum_{i<j}\Gamma_{ij} = 6\,(|\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{134}|^2 + |\Psi_{234}|^2) = 6 \tag{81}$$

Finally we can consider conditional probabilities, for example

$$p(1|2) = \frac{\Gamma_{12}}{n_2} = \frac{|\Psi_{123}|^2 + |\Psi_{124}|^2}{|\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{234}|^2} \tag{82}$$

We can further calculate the probability $p(1 \cup 2)$ that there is a particle in $\mathcal{I}_1$ or in $\mathcal{I}_2$. From the probability rule (see Eq.(A8) in the Appendix)

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) \tag{83}$$

we see that

$$\begin{aligned} p(1 \cup 2) &= n_1 + n_2 - \Gamma_{12} \\ &= (|\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{134}|^2) + (|\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{234}|^2) - (|\Psi_{123}|^2 + |\Psi_{124}|^2) \\ &= |\Psi_{123}|^2 + |\Psi_{124}|^2 + |\Psi_{134}|^2 + |\Psi_{234}|^2 = 1 \end{aligned} \tag{84}$$

This was to be expected since there is no multi-index I in which both labels 1 and 2 are missing, so we are sure to find a particle in either interval $\mathcal{I}_1$ or in $\mathcal{I}_2$.

E. Finite differencing for the many-particle Schrödinger equation

The finite differencing for the many-particle Schrödinger equation proceeds along similar lines as that for the one-particle case. We have an anti-symmetric wavefunction $\Psi(x_1, \dots, x_N)$ satisfying the Schrödinger equation

$$\left[-\frac{1}{2} \sum_{k=1}^{N} \frac{d^2}{dx_k^2} + u(x_1, \dots, x_N) \right] \Psi(x_1, \dots, x_N) = E\Psi(x_1, \dots, x_N) \tag{85}$$

where the potential u can be of general form in following, but is typically of the form

$$u(x_1, \dots, x_N) = \sum_{k=1}^{N} v(x_k) + \sum_{k<l}^{N} w(x_k, x_l) \tag{86}$$

for some external potential $v(x)$ and two-body interaction $w(x, x')$. We can write the Schrödinger equation as

$$(\hat{H}\Psi)(x_1, \dots, x_N) = E\Psi(x_1, \dots, x_N) \tag{87}$$

where $\hat{H} = \hat{T} + \hat{U}$ is the Hamilton operator and where the kinetic and potential energy operator are defined as:

$$(\hat{T}\varphi)(x_1, \dots, x_N) = -\frac{1}{2} \sum_{k=1}^{N} \frac{d^2\Psi}{dx_k^2} \qquad (\hat{U}\varphi)(x_1, \dots, x_N) = u(x_1, \dots, x_N)\Psi(x_1, \dots, x_N) \tag{88}$$

We following the same consideration as of the one-particle case. We employ for each of the coordinates x_k the boundary conditions

$$\Psi(x_1, \dots, x_{k-1}, 0, x_{k+1}, \dots, x_N) = 0 \qquad \Psi(x_1, \dots, x_{k-1}, L, x_{k+1}, \dots, x_N) = 0 \tag{89}$$

We take $\Delta L = L/(n+1)$ and discretise coordinate x_k by defining the lattice points $x_{i_k} = i_k \, \Delta L$ for $i_k \in \{1, \dots, N\}$. Let us now define

$$\Phi_I = \Psi(x_{i_1}, \dots, x_{i_N}) \qquad I = (i_1, \dots, i_N) \tag{90}$$

where at this point we do not require an ordering of the i_k yet. The action of the potential is simple as before

$$(\hat{U}\Psi)(x_{i_1}, \dots, x_{i_N}) = u(x_{i_1}, \dots, x_{i_N})\Psi(x_{i_1}, \dots, x_{i_N}) \tag{91}$$

Its action as a matrix on the vector Φ_I is then again given by a diagonal matrix of the form

$$U_{IJ} = \delta_{IJ} u_I \tag{92}$$

where we denoted $u_I = u(x_{i_1}, \dots, x_{i_N})$. To determine the action of the kinetic energy operators we again do the Taylor expansions:

$$\Psi(\dots x_{i_k+1} \dots) = \Psi(\dots x_{i_k} + \Delta L \dots) = \Psi(\dots x_{i_k} \dots) + \Delta L \frac{d\Psi}{dx_k}(\dots x_{i_k} \dots) + \frac{(\Delta L)^2}{2} \frac{d^2\Psi}{dx_k^2}(\dots x_{i_k} \dots) + \dots \tag{93}$$

$$\Psi(\dots x_{i_k-1} \dots) = \Psi(\dots x_{i_k} - \Delta L \dots) = \Psi(\dots x_{i_k} \dots) - \Delta L \frac{d\Psi}{dx_k}(\dots x_{i_k} \dots) + \frac{(\Delta L)^2}{2} \frac{d^2\Psi}{dx_k^2}(\dots x_{i_k} \dots) + \dots \tag{94}$$

where the dots denote the other coordinates that are kept fixed. As before we add both equations and neglect higher order terms and re-arrange to obtain

$$\frac{d^2\Psi}{dx_k^2}(\dots x_{i_k}\dots) = \frac{1}{(\Delta L)^2}\left[\Psi(\dots x_{i_k-1}\dots) - 2\Psi(\dots x_{i_k}\dots) + \Psi(\dots x_{i_k+1}\dots)\right]$$
$$= \frac{1}{(\Delta L)^2}(\Phi_{i_1\dots i_{k-1},i_k-1,i_{k+1}\dots i_N} - 2\Phi_{i_1\dots i_{k-1},i_k,i_{k+1}\dots i_N} + \Phi_{i_1\dots i_{k-1},i_k+1,i_{k+1}\dots i_N}) \tag{95}$$

It then follows that

$$-\frac{1}{2}\frac{d^2\Psi}{dx_k^2}(\dots x_{i_k}\dots) = \sum_{j_k=1}^{n} T_{i_k j_k}\Phi_{i_1\dots i_{k-1},j_k,i_{k+1}\dots i_N} \tag{96}$$

where T_{ij} is the matrix of Eq.(15). The kinetic energy is then given by

$$(\hat{T}\varphi)(x_{i_1}\dots,x_{i_N}) = \sum_{k=1}^{N}\sum_{j_k=1}^{n} T_{i_k j_k}\Phi_{i_1\dots i_{k-1},j_k,i_{k+1}\dots i_N} \tag{97}$$

such that the discretised Schrödinger equation becomes

$$\sum_{k=1}^{N}\sum_{j_k=1}^{n} T_{i_k j_k}\Phi_{i_1\dots i_{k-1},j_k,i_{k+1}\dots i_N} + u_{i_1\dots i_N}\Phi_{i_1\dots i_N} = E\Phi_{i_1\dots i_N} \tag{98}$$

This can be written as

$$\sum_J H_{IJ}\Phi_J = E\Phi_I \tag{99}$$

where here the sum goes over all indices J and not only over the ordered ones. If we define the matrix

$$H_{IJ} = T_{IJ} + U_{IJ} \tag{100}$$

where

$$T_{IJ} = \sum_{k=1}^{N}\delta_{i_1 j_1}\dots\delta_{i_{k-1}j_{k-1}}T_{i_k j_k}\delta_{i_{k+1}j_{k+1}}\dots\delta_{i_N j_N} \tag{101}$$

The expression (99) is the many-particle generalisation of the one-particle finite difference equation (19).

We will say a bit more later, but it is late on Friday now and I would also like to enjoy the weekend :-)

Appendix A: Probabilities

Here we give some basic relations related to the calculation of probabilities. A simple probabilistic experiment is given by a total set of outcomes Ω, like the numbers $\Omega = \{1,2,3,4,5,6\}$ that occurs as all possible outcomes from throwing a dice, and the set of events A of interest, like the set $A = \{4,5,6\}$ for throwing a number larger than 3 with a dice. For any given set S we denote by $|S|$ its number of elements. Then the probability $P(A)$ for an outcome in A is defined as

$$P(A) = \frac{|A|}{|\Omega|} \tag{A1}$$

This probability model is sometimes referred to as Laplace's rule for equiprobable events since the elementary events, i.e. sets containing a single element of Ω, are equally probable with probability $1/|\Omega|$. This models well the throw of a dice in which all single outcomes are equally likely with probability $1/6$. From Eq.(A1) we see that the probability of throwing larger than 3 is $P(A) = 3/6 = 1/2$. If we are given a second outcome set, like the set B of prime number in Ω, i.e. $B = \{2,3,5\}$, then we can

ask for the probability of throwing a prime number larger than 3, i.e. the probability that an event is both in A and in B. Since we have $A \cap B = \{4,5,6\} \cap \{2,3,5\} = \{5\}$ we find

$$P(A \cap B) = \frac{|A \cap B|}{|\Omega|} = \frac{1}{6} \tag{A2}$$

For two disjoint sets A and C with an empty intersection $A \cap C = \emptyset$, we have that the number of elements in their union $A \cup C$ is the sum of the number of elements in the separate sets, i.e.

$$|A \cup C| = |A| + |C| \tag{A3}$$

This describes mutually exclusive events, and in that case we have

$$P(A \cup C) = \frac{|A \cup C|}{|\Omega|} = \frac{|A| + |C|}{|\Omega|} = P(A) + P(C) \tag{A4}$$

and this is easily extended to any number of disjoint sets. For example let $C = \{1,2\}$ describe the events of throwing less than 3 with a dice. Then $P(C) = 2/6 = 1/3$ and for our other example set $A = \{4,5,6\}$ we have $A \cap C = \emptyset$ and therefore the probability for throwing a number that is either larger than three or lesser than three is given by $P(A) + P(C) = 1/2 + 1/3 = 5/6$. The main question now is how to calculate $P(A \cup B)$ when A and B are not disjoint. We derive this now and we start with some definitions. We let $A \setminus B$ the set of elements of A that are not in B. Since $A = (A \setminus B) \cup (A \cap B)$, where $A \setminus B$ and $A \cap B$ are disjoint, it follows from Eq.(A4) that

$$P(A) = P(A \setminus B) + P(A \cap B) \quad \Rightarrow \quad P(A \setminus B) = P(A) - P(A \cap B) \tag{A5}$$

Now we have

$$A \cup B = (A \setminus B) \cup (A \cap B) \cup (B \setminus A) \tag{A6}$$

where all the sets within round brackets on the right hand side are disjoint. It thus follows that

$$\begin{aligned} P(A \cup B) &= P(A \setminus B) + P(A \cap B) + P(B \setminus A) = (P(A) - P(A \cap B)) + P(A \cap B) + (P(B) - P(A \cap B)) \\ &= P(A) + P(B) - P(A \cap B) \end{aligned} \tag{A7}$$

where in the last step we used Eq.(A5) as well as that equation with A and B interchanged. For overlapping sets A and B expression (A4) is thus generalised to

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) \tag{A8}$$

We can apply this to our example sets A and B; the probability to throw a prime number or a number larger than three with a dice is given by

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) = \frac{1}{2} + \frac{1}{2} - \frac{1}{6} = \frac{5}{6} \tag{A9}$$

which we also could have calculated directly from the union $A \cup B = \{2,3,4,5,6\}$ and which indeed gives the same result as it should. Finally we consider conditional probabilities. We denote by $P(B|A)$ the probability of finding an outcome in B given that we have an outcome in A. This is clearly given by

$$P(B|A) = \frac{|A \cap B|}{|A|} = \frac{|A \cap B|/|\Omega|}{|A|/|\Omega|} = \frac{P(A \cap B)}{P(A)} \tag{A10}$$

In our example the probability of throwing a prime number, given that we know we threw a number larger than three, is $P(B|A) = 1/3$. We finally remark that by repeated application of Eq.(A8) we can calculate probabilities of unions for three and more overlapping sets. For example

$$\begin{aligned} P(A \cup B \cup C) &= P(A \cup B) + P(C) - P((A \cup B) \cap C) = P(A) + P(B) - P(A \cap B) + P(C) - P((A \cap C) \cup (B \cap C)) \\ &= P(A) + P(B) + P(C) - P(A \cap B) - (P(A \cap C) + P(B \cap C) - P((A \cap C) \cap (B \cap C))) \\ &= P(A) + P(B) + P(C) - P(A \cap B) - P(A \cap C) - P(B \cap C) + P(A \cap B \cap C) \end{aligned} \tag{A11}$$

This is a very short Mathematica code that illustrates how you can solve the 1-dimensional Schrödinger equation using the finite difference method described in the notes.
We take the example of an harmonic oscillator as we can check the result by comparing to the known analytic result.
We choose the following parameters

In[234]:=
```
n = 400;
L = 1.0;
ΔL = L / (n + 1);
ω = 100;
```

The grid points are given by the expression:

In[238]:=
```
x[i_] = i * ΔL;
```

The kinetic energy matrix is given by

In[239]:=
```
T = -0.5 (1 / ΔL) ^ 2 Table[KroneckerDelta[i, j + 1] -
      2 KroneckerDelta[i, j] + KroneckerDelta[i, j - 1], {i, 1, n}, {j, 1, n}];
```

while the potential energy matrix for the case of the harmonic oscillator is given by

In[240]:=
```
V = 0.5 ω ^ 2 Table[KroneckerDelta[i, j] * (x [i] - L / 2) ^ 2, {i, 1, n}, {j, 1, n}];
```

and the Hamiltonian H is simple the sum of both matrices:

In[241]:=
```
H = T + V;
```

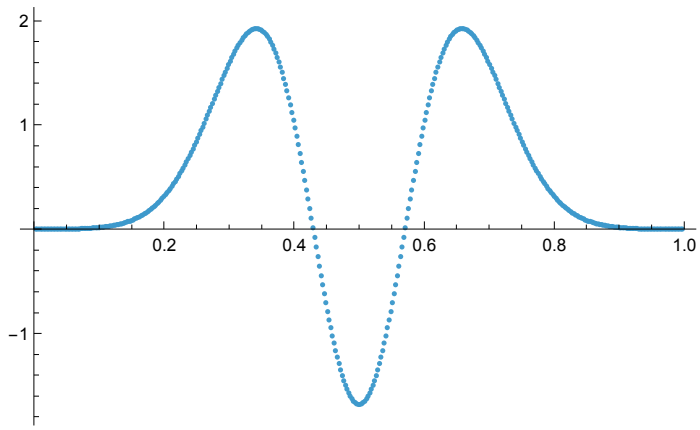
Then we calculate the eigenvectors by diagonalisation of H and normalise them such that the Riemann sum of the squared wavefunctions sums to one. For the normalisation used in Mathematica this requires division by the square root of ΔL. We store eigenvectors in a new matrix called Eigmat:

In[242]:=
```
Eigmat = Eigenvectors[H] / Sqrt[ΔL];
```

Now everything is done and we can plot. We plot below, as an example, the second excited state. Since Mathematica orders the n eigenvectors with the highest eigenvalue first, the second excited state
corresponds to label n-2:

In[243]:=
```
ListPlot[Table[{x[j], Eigmat[[n - 2, j]]}, {j, 1, n}]]
```

Out[243]=



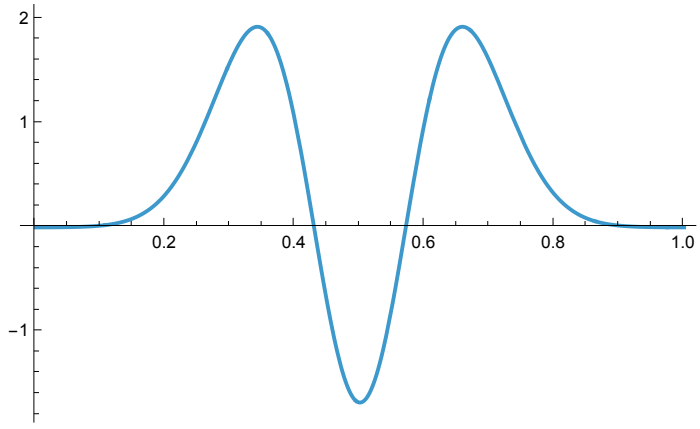
We can now compare this result to the known analytic solutions for the normalised harmonic oscillator eigenfunctions. The m-th normalised eigenstate is given by:

In[244]:=
```
ψ[m_, x_] := (ω / Pi) ^ (1 / 4) Exp[-0.5 ω (x - L / 2) ^ 2]
   HermiteH[m, Sqrt[ω] (x - L / 2)] (1 / Sqrt[(2 ^ m) Factorial[m]]);
```

and we plot the second excited state, i.e. we choose m=2:

In[245]:=
```
Plot[ψ[2, x], {x, 0, L}]
```

Out[245]=



By comparing the result we see that the finite difference solution is a very good approximation to the analytical solution.