Numerical Solutions to Eigenvalue Problems

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***Abstract*—The Jacobi method was used to find eigenvalues of various tridiagonal symmetric matrices. Eigenvalues were found for three different physical systems: A buckling beam, one electron in a harmonic oscillator, and two electrons in a harmonic oscillator with Coulomb interaction. All systems had second order differential equations which were discretized and represented as matrices. The eigenvalues of these matrices were found.**

For the buckling beam, the first 9 eigenvalues were found after 143 Jacobi rotations with high precision, and a very fast run time of 0.00026 seconds.

The eigenvalues for the one electron system were found with multiple different matrix dimensions, and the best results were 2.99987, 6.99937, 10.9985 and 14.9972 (compared with the analytic eigenvalues 3, 7, 11, 15,...), this was for an 499x499 matrix which took 743 seconds to calculate.

For the two electron system, the eigenpairs for the ground state were found and the results were illustrated by plotting the probability distribution for various oscillator frequencies. The results reveal that if the strength of the potential increases, then the uncertainty of position decreases.

I. Introduction

Finding the eigenvalues of a matrix efficiently has long been a major topic in numerical linear algebra. There are various methods designed to do this and the methods vary greatly in accuracy and computation time. Finding the balance between these two is one of the several themes presented in the report. Three specialized physics cases are presented and solved numerically using *Jacobi's method*, a method widely used to calculate the eigenpairs (eigenvectors and their corresponding eigenvalues). These eigenpairs are then used to describe the various states and solutions to the systems. The problems were a compressed buckling beam and two quantum mechanical systems: one electron in a harmonic oscillator and two electrons in a harmonic oscillator with Coulomb interaction.

The Jacobi method is an algorithm used to determine eigenpairs in diagonally dominated matrices; using this method to solve the three systems presented involves discretization of second order differential equations and describing them in terms of tridiagonal matrices. The three systems had major similarities to them, meaning they could be solved in mostly the same fashion with some variations in scaling. Due to the similarity of the systems, all three cases were solved using the generalized *Jacobi method*. Though the presented cases are specific, the same solutions can be applied to several other fields of research such as meteorology, engineering and electrostatics by only small modifications of the equations.

The report presented is designed to introduce the reader to the theoretical models describing the phenomena with a *theory* section before presenting *Jacobi method* and other techniques used to produce accurate results in the *method* section. Afterwards, a discussion of the results is conducted and utilized to produce meaningful conclusions to the research.

The report, algorithm and other analyses calculations were all developed and solved in cooperation by Steinn Hauser and Simen Håpnes. The scripts and some text file examples of results were all uploaded to the following shared github repository (linked):
https://github.com/steinnhauser/FYS3150/tree/master/Project2

II. Theory

Consider a buckling beam oriented horizontally along the x axis, fastened to an immovable wall at points $x = 0$ and $x = L$. This means that the beam is fixed at the boundary points, and the rest of the beam is allowed to move up and down in the y-direction.

Let the vertical displacement at each point $x \in (0, L)$ be $u(x)$ and let there be a force F from point $(x = L, y = 0)$ with a direction towards the origin. This force compresses the beam and sets it into a buckling motion (the beam is quite incompressible). The vertical displacement of the mass is then described by the differential equation

$$\gamma \frac{\mathrm{d}^2 u(x)}{\mathrm{d}x^2} = -Fu(x), \tag{1}$$

where γ is a material constant (characteristic of the beam) in Nm^2, and F is the force applied in N. This equation can be scaled and generalized to fit multiple systems in the following fashion:

$$\frac{\mathrm{d}^2 u(\rho)}{\mathrm{d}\rho^2} = -\lambda u(\rho) \tag{2}$$

This scaled differential equation is described by a unitless distance variable $\rho = x/L$, which is a natural length scale for the system and $\rho \in (0, 1)$. The relation $\lambda = FL^2/\gamma$ applies to the case of the buckling beam, but other second order differential equations will utilize a different λ definition.

Consider now a new system of electrons caught in a potential, the one electron system is in a harmonic oscillator (HO) potential, and the two electron system is in a *Coulumb* and *HO* potential. The radial part of Schrödinger's equation is then described by

$$\hat{H}R(r) = ER(r), \tag{3}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2}\right) + V, \tag{4}$$

where V is the potential energy and m is the particle's mass in kg. This equation uses a spherical coordinate system where r is the distance from the center in m. Assuming the angular momentum quantum number $l = 0$ produces the relation:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r}\right)R(r) + V(r)R(r) = ER(r) \tag{5}$$

This expression can be simplified by utilization of a function $u(r) = R(r)/r$, such that the boundary conditions become

$u(0) = 0$ and $u(\infty) = 0$. The Schrödinger equation now reads:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u}{\mathrm{d}r^2} + V(r)u(r) = Eu(r) \tag{6}$$

Further generalization is achieved by implementing a dimensionless distance variable ρ as done in the previous case of the buckling beam.

The Schrödinger equation will be utilized to simulate the behaviour of one electron in a HO potential and two electrons in a HO and Coulomb potential. The one electron system has analytic eigenvalues, were the first four are $\lambda = 3, 7, 11, 15, \ldots$.

For the two electron system, the potential energy $V(r)$ for the system can be described by the sum of the *Coulumb* and *Harmonic Oscillator* potentials:

$$V(\rho) = V_{HO}(\rho) + V_C(\rho) = \omega_r^2\rho^2 + \frac{1}{\rho} \tag{7}$$

ω_r is the angular frequency, and ρ is the unitless radial parameter expressed by $\rho = r/\alpha$ (a natural length scale for this system). α and r have unit length. $r \in [0, \infty]$ and $\alpha = \hbar^2/(m \cdot 1.44eVnm)$. The parameter α is adjusted such that the potential expressions are concise and easy to handle. The maximal value of r must be asserted as $r = \infty$ is not sufficient, this will be further discussed in later sections.

III. Method

The goal with *the Jacobi method* for the buckling beam and one electron systems was to find the eigenvalues, representing the stable states. These two systems have analytic eigenvalues which are very useful when checking for calculation errors and when performing a meaningful error analyses.

The two electron system was studied a bit further, where the eigenpairs were used to look at the wave function in the ground state (lowest energy state). This was done for several different angular frequencies ω_r to visualize what consequences the potential strength had on the wave function.

A. The Jacobi Method

Suppose an orthogonal matrix $\hat{S}$, corresponding to a linear transformation which rotates a basis by an angle θ. This matrix is then described (in two dimensions) by:

$$\hat{S} = \begin{bmatrix} cos(\theta) & sin(\theta) \\ -sin(\theta) & cos(\theta) \end{bmatrix} \tag{8}$$

This matrix will rotate any vector or basis in the two dimensional plane by an angle θ around the origin. This orthogonal transformation has the characteristic of preserving the orthogonality and length of transformed vectors; assume an orthonormal (orthogonal and normalized) basis consisting of vectors $[\hat{u}_1, \hat{u}_2, \hat{u}_3, \ldots]$ which share the property of:

$$\hat{u}_i^\top \hat{u}_j = \delta_{i,j} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases} \tag{9}$$

This can be used to formalize the preservation of orthonormality as mentioned above. Now assume a new basis of vectors $[\hat{v}_1, \hat{v}_2, \hat{v}_3, \ldots]$ which has a relation to the basis $\hat{u}_i$ described by:

$$\hat{v}_i = \hat{S}\hat{u}_i \tag{10}$$

Utilizing that the matrix $\hat{S}$ is an orthogonal matrix, possessing the properties

$$\hat{S}^\top \hat{S} = \hat{S}\hat{S}^\top = \hat{I} \tag{11}$$

allows for the conclusion of:

$$\hat{v}_i^\top \hat{v}_j = \hat{u}_i^\top \underbrace{\hat{S}^\top \hat{S}}_{\mathrm{I}} \hat{u}_j = \hat{u}_i^\top \hat{u}_j = \delta_{ij} \tag{12}$$

In other words, the matrix $\hat{S}$ preserves the orthonormality of vectors. This property is utilized in *the Jacobi method* to calculate the eigenvalues λ of some real $n \times n$ matrix $\hat{A}$:

$$\hat{A}\hat{u} = \lambda\hat{u} \Rightarrow \hat{S}\hat{A}\hat{u} = \hat{S}\lambda\hat{u} \tag{13}$$

Inserting an identity matrix $\hat{I} = \hat{S}^\top\hat{S}$ between $\hat{A}$ and $\hat{u}$ returns:

$$\hat{S}\hat{A}\hat{S}^\top(\hat{S}\hat{u}) = \lambda(\hat{S}\hat{u}) \Rightarrow \hat{D}(\hat{S}\hat{u}) = \lambda(\hat{S}\hat{u}) \tag{14}$$

The matrix $\hat{D}$ is a diagonal matrix which consists of the eigenvalues corresponding to the eigenvectors of $\hat{A}$:

$$\hat{D} = \begin{bmatrix} \lambda_1 & 0 & 0 & \ldots & 0 \\ 0 & \lambda_2 & 0 & \ldots & 0 \\ 0 & 0 & \lambda_3 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & \lambda_{n-1} \end{bmatrix} \tag{15}$$

This eigenvalue matrix is what *the Jacobi method* is utilized to calculate numerically for a given $n \times n$ matrix $\hat{A}$. The method utilizes the orthogonal rotation matrix $\hat{S}$ in an attempt to reduce the non-diagonal elements of the matrix $\hat{A}$ to zero. What's left (when the non-diagonal elements are sufficiently low) is the eigenvalues along the diagonal as the result of the calculation.

Doing this numerically involves performing the rotation $\hat{S}$ specifically around a non-diagonal element in the $\hat{A}$ matrix, and choosing the rotation angle θ such that the element is set to zero. Doing this multiple times for the non-diagonals eventually produces an accurate approximation of the diagonal eigenvalue matrix $\hat{D}$ numerically.

Choosing which non-diagonal element to rotate about often depends on circumstance, as the variants can often have a large impact on the runtime of the program. The variant of *Jacobi's method* chosen for this case is the *general Jacobi's method*, which locates the largest non-diagonal matrix element and rotates about it (such that it equals zero afterwards). This process is repeated until the absolute value of all non-diagonal elements are smaller than a tolerance (the tolerance was varied, but was between 10^{-16} and 10^{-10}), meaning that they are all approximately zero. Other variants of *the Jacobi method* (such as the cyclic *Jacobi*) are not compared in this report.

The *general Jacobi method* algorithm is written in C++ and consists of three central objectives for each iteration; it locates the largest (in absolute value) non-diagonal element, calculates the optimal rotation angle θ, and applies the rotation such that the element is set to zero. The

mathematical equation for the optimal rotation angle θ for the element given by indexes a_{kl} is given by:

$$cot(2\theta) = \tau = \frac{a_{ll} - a_{kk}}{2a_{kl}} \tag{16}$$

The indexes l and k represent the coordinates of the maximum non-diagonal element of the matrix. This allows us to obtain the quadratic equation (by the relation $cot2\theta = (cot\theta - tan\theta)/2$)

$$t^2 + 2\tau t - 1 = 0, \tag{17}$$

which is solvable for t ($t = \tan(\theta)$) by the following equation:

$$t = -\tau \pm \sqrt{1 + \tau^2} \tag{18}$$

Once the t value is calculated, the cosine (c) and sine (s) values can also be obtained by the trigonometric relations:

$$c = \frac{1}{\sqrt{1 + t^2}}, \; s = tc \tag{19}$$

These values of c and s allows us to build the rotation matrix $\hat{S}$ which is utilized to rotate $\hat{A}$ and set its largest element to zero. These steps are then repeated for the next largest non-diagonal element of $\hat{A}$ until all non-diagonal elements effectively equal zero. This is the essence of the algorithm, finally producing an approximation of the diagonal matrix $\hat{D}$ described in equation 15. The accuracy of this approximation depends on how small or large the tolerance is, as explained earlier.

B. Application to differential equations

This eigenpair matrix analyses can be applied to the buckling beam and quantum systems presented in previous sections; this is done by *discretization* and *Taylor expansion*. The differential equation 2 can be rewritten and discretized (through *Taylor expansion*, see appendix A) as:

$$u_i'' = -\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} \tag{20}$$

Where h is the step length, and $i = 1, 2, 3, ..., N-1$ (the end points describe the boundary conditions). These types of equations can be written as the following symmetric tridiagonal matrix multiplication:

$$\begin{bmatrix} d & a & 0 & \dots & 0 \\ a & d & a & \dots & 0 \\ 0 & a & d & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & a \\ 0 & 0 & 0 & a & d \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \\ \vdots \\ \\ u_{N-1} \end{bmatrix} = \lambda \begin{bmatrix} u_1 \\ u_2 \\ \\ \vdots \\ \\ u_{N-1} \end{bmatrix} \tag{21}$$

For equation 20, the diagonal elements will be, $d = 2/h^2$ and $a = -1/h^2$. This type of tridiagonal Töeplitz matrix has analytical eigenvalues[1]:

$$\lambda_j = d + 2a\cos\left(\frac{j\pi}{N+1}\right) \tag{22}$$

where $j = 1, 2, 3, ..., N-1$. which means there are just as many eigenpairs as elements as the matrix dimension. The buckling beam problem was solved dimensionless, and the method can be extended to solve more general problems.

Utilizing the same method for the Schrödinger equation described in equation 6 simply involves manipulating the diagonal matrix elements of $\hat{A}$ in the same fashion such that the potential $V(\rho)$ (from equation 7) is also included. Since the potential now depends on the position of the electron, the matrix $\hat{A}$ has the following form:

$$\hat{A} = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & \dots & 0 \\ 0 & -1 & 2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} + \hat{V} \tag{23}$$

$$\hat{V} = \begin{bmatrix} V(\rho_1) & 0 & 0 & \dots & 0 \\ 0 & V(\rho_2) & 0 & \dots & 0 \\ 0 & 0 & V(\rho_3) & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & 0 & V(\rho_{n-1}) \end{bmatrix} \tag{24}$$

The potential V is different for the one electron and two electron systems. For one electron, the potential consists of the *Harmonic oscillator* potential $V(\rho_i) = \omega_r^2\rho_i^2$, and for the two electron system, the *Coulomb potential* is also included: $V(\rho_i) = \omega_r^2\rho_i^2 + (1/\rho_i)$, where $i = 1, 2, 3, \dots, n-1$.

IV. Results

A. The Buckling Beam

In table I the analytic eigenvalues and numerical eigenvalues are listed and compared. The analytic ones were found using equation 22.

TABLE I
EIGENVALUES FOR THE BUCKLING BEAM, SOLVED NUMERICALLY WITH A 9×9 MATRIX AND THE JACOBI METHOD. THE CALCULATIONS TOOK $0.000261s$ AND 143 ITERATIONS BEFORE COMING WITHIN THE TOLERANCE $\epsilon = 1e-8$.

Analytic eigenvalues	Numerical eigenvalues
9.7887	9.7887
38.1966	38.1966
82.4429	82.4429
138.197	138.197
200	200
261.803	261.803
317.557	317.557
361.803	361.803
390.211	390.211

B. One electron system

By using a different size matrices, the first four eigenvalues (lowest four) were found. Table II shows the analytic eigenvalues as well as numerical eigenvalues for different matrix dimensions.

TABLE II
ANALYTIC VALUES, AND NUMERICAL EIGENVALUES CALCULATED BY *Jacobi's method* USING DIFFERENT MATRIX DIMENSIONS $n \times n$.

Analytic eigvals	$n = 199$	$n = 299$	$n = 399$	$n = 499$
3	2.99922	2.99965	2.9998	2.99987
7	6.99609	6.99826	6.99902	6.99937
11	10.9905	10.9958	10.9976	10.9985
15	14.9823	14.9921	14.9956	14.9972
time	13.8105	84.6468s	280.304s	742.985
iterations	63410	144732	259167	407112

Following are the relative error percentages from table II for the same matrix dimentions:

TABLE III
RELATIVE ERROR ANALYSES (IN %) FROM TABLE II. THE ERRORS WERE CALCULATED BY COMPARISON TO THE ANALYTIC RESULTS LISTED.

	Relative Error [%]			
Analytic eigvals	$n = 199$	$n = 299$	$n = 399$	$n = 499$
3	0.026	0.012	0.0067	0.0043
7	0.056	0.025	0.014	0.009
11	0.086	0.038	0.022	0.014
15	0.118	0.053	0.029	0.019

C. Two electron system

Figure 1 shows the probability distribution of the ground state vs. distance between the two electrons (as a unitless natural length scale), for different oscillator frequencies.

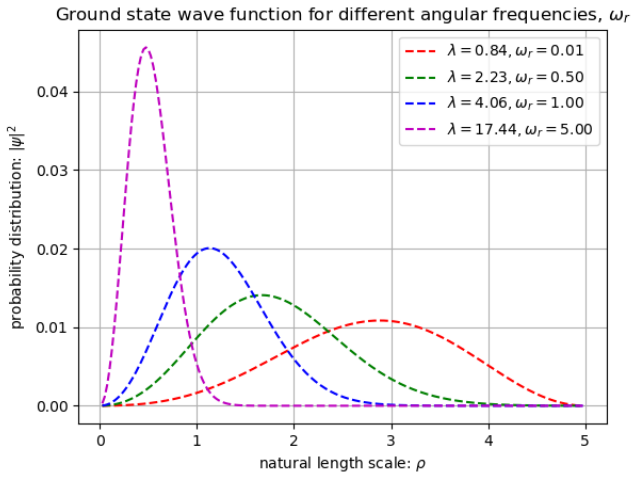

Fig. 1. Probability distribution (the norm squared of the wavefunctions, which is then eigenvector) vs. ρ, for different oscillator frequency strengths. The values indicate a probability distribution of where the electron is most likely located. The maximum natural length scale chosen for this system was $\rho_{max} = 5$, such that $u(0) = u(5) = 0$.

V. DISCUSSION

A. The Buckling Beam

Table I illustrates the accuracy of *Jacobi's method*. The numerical eigenvalues match with the analytic predictions by 12 decimal points after 143 iterations with 9 integration points. This accuracy is very impressive considering the small tolerance $\epsilon = 10^{-8}$; increasing this tolerance did not increase the accuracy very much in this case, but increased the computation time unnecessarily. How accurate these results are to a real world buckling beam is more questionable seeing as the discretization of $x \in (0, L)$ only included 9 mesh grid points. This large mesh grid approximation would likely produce noticeable numerical errors for larger values of L.

B. One Electron System

Table II is a good example of the accuracy increase for larger values of N. The smallest eigenvalues are noticeably the most accurate, even when considering the relative error. Why it is so is uncertain but lies somewhere in the objective of the algorithm. There were two main approaches to increasing the accuracy: making the tolerance for the largest non-diagonal element smaller (between 10^{-8} and 10^{-16}) or increasing the matrix dimension n. However, both methods led to a large increment in computational time for the program. The most influential to the computation time was the matrix dimension, as can be seen from table II. The largest matrix dimension used was a 499×499 matrix with the most effective zero tolerance of 10^{-8} (this took 743 seconds, and used 407,112 rotations). This led to a precision of four decimal points for the lowest eigenvalue (2.99987). Such a precision increase was however not worth the computation time. It took the program 14 seconds to calculate the 199×199 matrix and the value of the smallest eigenvalue was only off by 0.00078.

Interestingly enough, the relative errors seem to increase linearly with the analytic eigenvalues. This indicates to some fault in *Jacobi's method* which is related to increasing values of λ. Why this is is uncertain but it would be interesting to dive into a deeper error analyses for tables II and III.

C. Two Electron System

Figure 1 shows that for larger angular frequencies ω_r, the relative distance $r = \rho\alpha$ between the electrons becomes smaller. According to (Taut, M: 1993)[2] the system should reach its natural length scale as the harmonic oscillator potential decreases ($\omega_r \to 0 \Rightarrow \rho \to 1$). The explanation for this is that when the oscillator energy decreases, the Coulomb interaction should dominate, and hence should the electrons approach their natural distance.

Another property shown by figure 1 is that the variance of the wave function seems to decrease with higher frequency, which indicates a less positional uncertainty. This may be related to Heisenberg's uncertainty principle in the sense that the momentum of the electron may have a larger uncertainty for larger values of ω_r.

VI. CONCLUSION

The Jacobi method found the eigenvalues for the buckling beam system and were extremely accurate for a low number of iterations. This was likely due to the small dimension of the matrix, being only $9x9$. For the one electron system, the first four eigenvalues approached the analytic eigenvalues with higher matrix dimension (more integration points). The relative error was lowest for the lowest eigenvalue, and increased with higher eigenvalues. The tolerance ϵ turned out not to have much of an influence when decreased under $\epsilon = 10^{-8}$, where the number of mesh grid points n were the dominant factor when deciding accuracy and computation time. In other words, though the errors decreased regularly as the number of mesh grid points increased, it was the exponential increase in run time which caused the accuracy to be limited. The two electron system had results which were difficult to interpret; the superposition of the electron wave functions (produced the results shown in figure 1) seems to decrease as the harmonic oscillator potential increases. This means that the relative distance between the electrons goes towards zero as the well strength pushes them together. This makes sense though the Columb potential should push them apart as a result. Perhaps this is what happens although it is difficult to see from the figure. All in all a solid computational method which produced excellent results.

. APPENDIX A: TAYLOR TRICKS

The Taylor expansion for a function $u(x)$ with a small step size h is as follows:

$$u(x \pm h) = u \pm hu^{(1)} + \frac{h^2}{2!}u^{(2)} \pm \frac{h^3}{3!}u^{(3)} + O(h^4) \quad (25)$$

The notation $u^{(n)}$ indicates the n-th derivative of the function u, and the last term $O(h^4)$ represents the error of the approximation. In this case the error is proportional to the step size to the fourth power $O(h^4) \sim h^4$. A combination of two such expansion results in the following:

$$u(x+h) + u(x-h) = 2u(x) + \frac{2}{2!}h^2u^{(2)} + O(h^4) \quad (26)$$

Rewriting this expansion returns the following result:

$$u^{(2)} = \frac{u(x+h) - 2u(x) + u_{(x-h)}}{h^2} + O(h^4) \quad (27)$$

Utilizing the discretized notation $u(x_i \pm h) = u_{i\pm1}$ returns:

$$u^{(2)} = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + O(h^4) \quad (28)$$

This can be rewritten to a vector-matrix multiplication by the two following expressions being equivalent (given the boundary conditions $u_0 = u_n = 0$):

i=1 $\quad u_1^{(2)} = (u_0 - 2u_1 + u_2)/h^2$
i=2 $\quad u_2^{(2)} = (u_1 - 2u_2 + u_3)/h^2$
i=3 $\quad u_3^{(2)} = (u_2 - 2u_3 + u_4)/h^2$
$\vdots$
i=n-1 $\quad u_{n-1}^{(2)} = (u_n - 2u_{n-1} + u_{n-2})/h^2$

$$\begin{bmatrix} u_1^{(2)} \\ u_2^{(2)} \\ u_3^{(2)} \\ \vdots \\ u_{n-1}^{(2)} \end{bmatrix} = \frac{1}{h^2} \begin{bmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ 0 & 1 & -2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{n-1} \end{bmatrix} \quad (29)$$

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