DTS104TC
NUMERICAL METHODS

LECTURE 3

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CONTENTS

- Special Matrices
- Iterative Methods (syllabus c)
- Summary of Methods for Linear Algebraic Equations

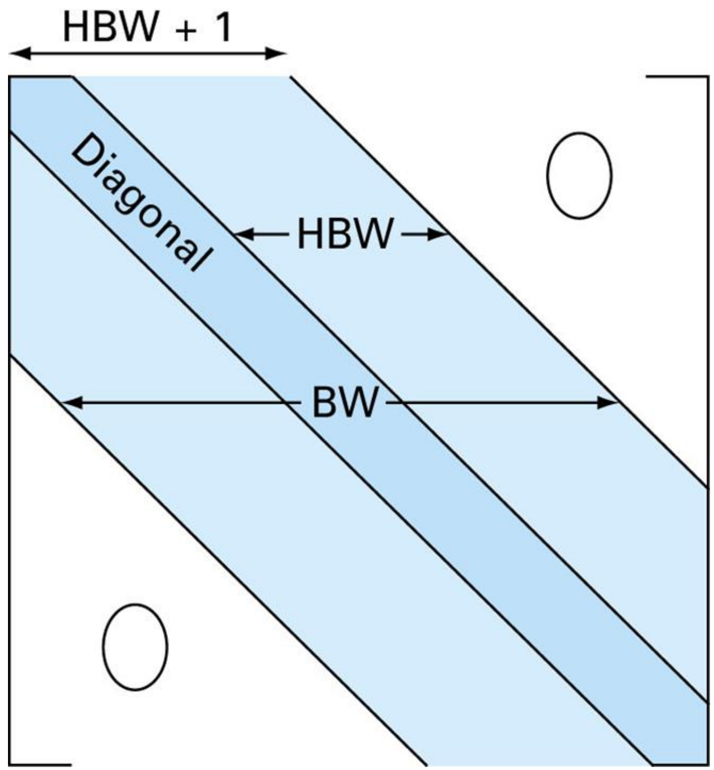
BANDED MATRICES

Certain matrices have particular structures that can be exploited to develop efficient solution schemes.

- A *banded matrix* is a square matrix that has all elements equal to zero, with the exception of a band centered on the main diagonal. These matrices typically occur in solution of differential equations.
- The dimensions of a banded system can be quantified by two parameters: the band width BW and half-bandwidth HBW. These two values are related by BW = 2HBW + 1.

- Methods like Gauss elimination are often inefficient in solving banded matrices for cases where pivoting is unnecessary because none of the elements outside the band would change from their original values of zero. Thus, unnecessary space and time would be expended on the storage and manipulation of these useless zeros.

BANDED MATRICES



- BW and HBW designate the bandwidth and the half-bandwidth, respectively.

TRIDIAGONAL SYSTEMS

$$
\begin{bmatrix}
f_1 & g_1 & & & & & \\
e_2 & f_2 & g_2 & & & \mathbf{0} & \\
 & e_3 & f_3 & g_3 & & & \\
 & & \cdot & \cdot & \cdot & & \\
 & & & \cdot & \cdot & \cdot & \\
 & \mathbf{0} & & & \cdot & \cdot & \cdot \\
 & & & & e_{n-1} & f_{n-1} & g_{n-1} \\
 & & & & & e_n & f_n
\end{bmatrix}
\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{Bmatrix}
=
\begin{Bmatrix} r_1 \\ r_2 \\ r_3 \\ \cdot \\ \cdot \\ \cdot \\ r_{n-1} \\ r_n \end{Bmatrix}
$$

THE THOMAS L U ALGORITHM (LU DECOMPOSITION VERSION)

- The Thomas Algorithm, which can be expressed as an *LU* decomposition method, can be used to efficiently solve tridiagonal systems. The algorithm consists of three steps: decomposition, forward and back substitution, and has all the advantages of *LU* decomposition.

(*a*) Decomposition

```
DOFOR k = 2, n
  e_k = e_k / f_(k-1)
  f_k = f_k - e_k · g_(k-1)
END DO
```

(*b*) Forward substitution

```
DOFOR k = 2, n
  r_k = r_k - e_k · r_(k-1)
END DO
```

(c) Back substitution

```
x_n = r_n / f_n
DOFOR k = n -1, 1, -1
  x_k = (r_k - g_k · x_(k+1))/f_k
END DO
```

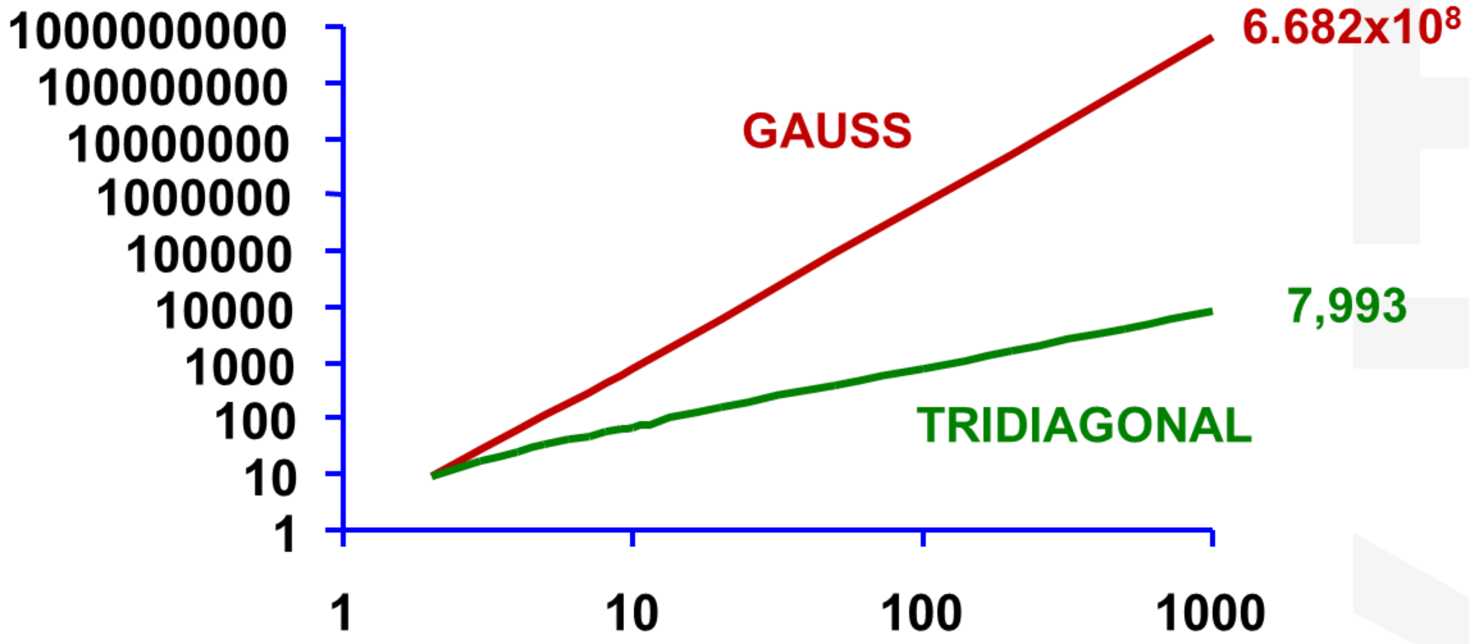
FLOPS

GAUSS ELIMINATION:

$$\frac{2n^3}{3}+O\left(n^2\right)$$

THOMAS ALGORITHM:

$$8n-7$$



JACOBI METHOD

- Iterative or approximate methods provide an alternative to the elimination methods. The Jacobi method is a form of fixed point iteration for a system of equations.

- The system $[A]\{x\}=\{b\}$ is reshaped by solving the first equation for x_1, the second equation for x_2, and the third for x_3, …and n^{th} equation for x_n. For conciseness, we will limit ourselves to 3×3 or 2×2 set of equations.

JACOBI METHOD

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

$$x_2 = \frac{b_2 - a_{21}x_1 - a_{23}x_3}{a_{22}}$$

$$x_3 = \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}}$$

- Now we can start the solution process by choosing guesses for the *x*'s. A simple way to obtain initial guesses is to assume that they are zero.

JACOBI METHOD

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$x_1 = \frac{b_1 - \cancelto{0}{a_{12}x_2} + \cancelto{0}{a_{13}x_3}}{a_{11}}$$

$$x_1 = \frac{b_1}{a_{11}}$$

- Do the same for x_2 and x_3
- Use the set of x_1, x_2 and x_3 for the next step

GAUSS-SEIDEL

- The Gauss-Seidel method is the most commonly used iterative method.

- The system $[A]\{x\}=\{b\}$ is reshaped by solving the first equation for x_1, the second equation for x_2, and the third for x_3, …and n^{th} equation for x_n. For conciseness, we will limit ourselves to 3×3 or 2×2 set of equations.

GAUSS-SEIDEL

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

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- Now we can start the solution process by choosing guesses for the *x*'s. A simple way to obtain initial guesses is to assume that they are zero.

GAUSS-SEIDEL

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$x_1 = \frac{b_1 - a_{12}\cancelto{0}{x_2} - a_{13}\cancelto{0}{x_3}}{a_{11}}$$

$$x_1 = \frac{b_1}{a_{11}}$$

GAUSS-SEIDEL

- New x_1 is substituted to calculate x_2 and x_3.
- New x_2 is substituted to x_3.
- New x_3 is substituted to x_1 in the next step.

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

$$x_2 = \frac{b_2 - a_{21}x_1 - a_{23}x_3}{a_{22}}$$

$$x_3 = \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}}$$

GAUSS-SEIDEL VERSUS JACOBI

Gauss-Seidel

Jacobi

First Iteration

Gauss-Seidel:

$$x_1 = (b_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$

$$x_2 = (b_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$

$$x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

Jacobi:

$$x_1 = (b_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$

$$x_2 = (b_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$

$$x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

Second Iteration

Gauss-Seidel:

$$x_1 = (b_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$

$$x_2 = (b_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$

$$x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

Jacobi:

$$x_1 = (b_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$

$$x_2 = (b_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$

$$x_3 = (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

SUCCESSIVE OVER-RELAXATION (SOR)

- Takes the Gauss-Seidel direction toward the solution and "overshoot" to try to speed convergence.

- Let ω be a real number, at step k+1

$$x_{1,k+1} = (1-\omega)x_{1,k} + \omega(\frac{b_1 - a_{12}x_{2,k} - a_{13}x_{3,k}}{a_{11}})$$

$$x_{2,k+1} = (1-\omega)x_{2,k} + \omega(\frac{b_2 - a_{21}x_{1,k+1} + a_{23}x_{3,k}}{a_{22}})$$

$$x_{3,k+1} = (1-\omega)x_{3,k} + \omega(\frac{b_3 - a_{31}x_{1,k+1} + a_{32}x_{2,k+1}}{a_{22}})$$

- No general theory on deciding ω. Some discussion available for common special cases.

CONVERGENCE

- New x_1 is substituted to calculate x_2 and x_3. The procedure is repeated until the convergence criterion is satisfied:

$$\left|\varepsilon_{a,i}\right| = \left|\frac{x_i^j - x_i^{j-1}}{x_i^j}\right| 100\% < \varepsilon_s$$

- For all *i*, where *j* and *j* – 1 are the present and previous iterations.
- Gauss-Seidel, like Jacobi, converges to the solution as long as the coefficient matrix is strictly diagonally dominant.

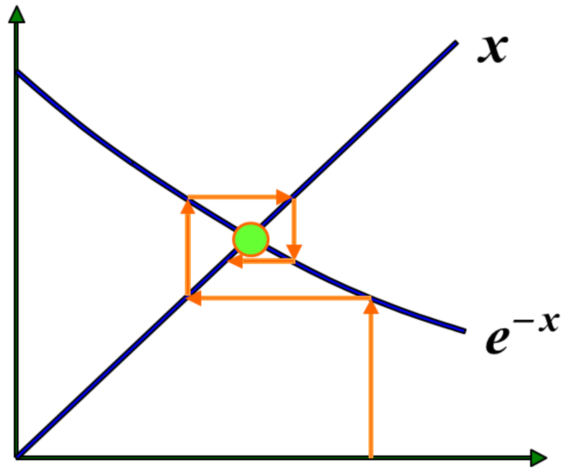
CONVERGENCE CRITERION FOR GAUSS-SEIDEL METHOD

The Gauss-Seidel method has two fundamental problems as with any iterative method:

- It is sometimes nonconvergent, and
- If it converges, can converge very slowly.

RECALL FIXED-POINT ITERATION

$$x_{i+1} = g(x_i)$$



$$E_{i+1} = g'(\xi)E_i$$

$$\left|\frac{\partial g}{\partial x}\right| < 1$$

GAUSS-SEIDEL AS A FIXED POINT ITERATION

$$x_1 = \frac{b_1 - a_{12}x_2}{a_{11}}$$

$$x_2 = \frac{b_2 - a_{21}x_1}{a_{22}}$$

$$x_1 = g_1(x_1, x_2)$$

$$x_2 = g_2(x_1, x_2)$$

CONVERGENCE CRITERIA

$$\left|\frac{\partial g_1}{\partial x_1}\right| + \left|\frac{\partial g_2}{\partial x_1}\right| < 1$$

$$\left|\frac{\partial g_1}{\partial x_2}\right| + \left|\frac{\partial g_2}{\partial x_2}\right| < 1$$

$$\frac{\partial g_1}{\partial x_1} = 0$$

$$\frac{\partial g_1}{\partial x_2} = \frac{a_{12}}{a_{11}}$$

$$\frac{\partial g_2}{\partial x_1} = \frac{a_{21}}{a_{22}}$$

$$\frac{\partial g_2}{\partial x_2} = 0$$

$$\left|\frac{a_{21}}{a_{22}}\right| < 1$$

$$\left|\frac{a_{12}}{a_{11}}\right| < 1$$

DIAGONAL DOMINANCE

$$\left|\frac{a_{21}}{a_{22}}\right| < 1 \qquad \left|\frac{a_{12}}{a_{11}}\right| < 1$$

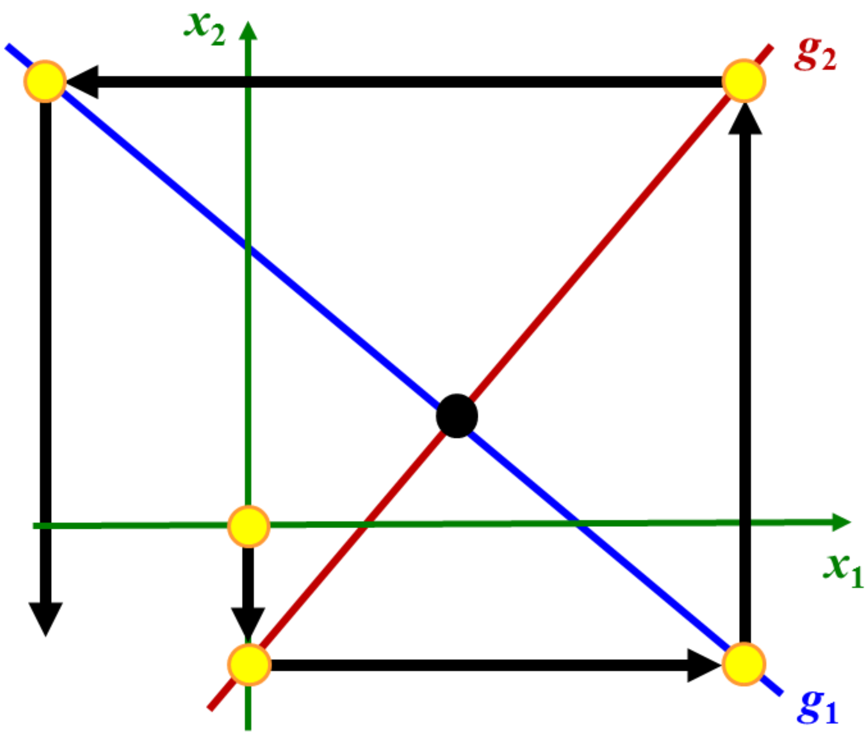
$$|a_{22}| > |a_{21}|$$
$$|a_{11}| > |a_{12}|$$

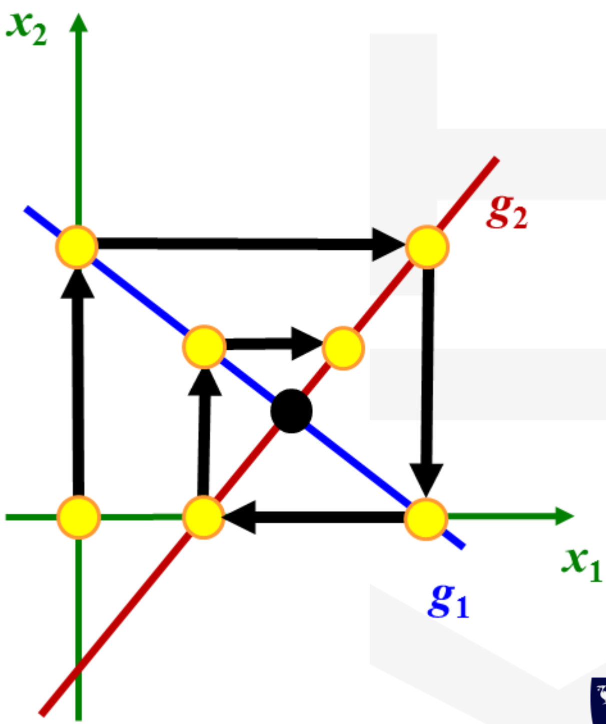
The absolute value of the diagonal coefficient in each of the equations must be larger than the sum of the absolute values of the other coefficients in the equation.

DIAGONAL DOMINANCE

$$g_2(x_1,x_2):\ 11x_1+13x_2=286$$
$$g_1(x_1,x_2):\ 11x_1-9x_2=99$$

$$g_1(x_1,x_2):\ 11x_1-9x_2=99$$
$$g_2(x_1,x_2):\ 11x_1-13x_2=286$$





HOW TO DEAL WITH IT

- Many physically-based models are naturally diagonally dominant.
- If not, rearrange equations.

$$\begin{bmatrix} 1 & -2 & -4 & 9 \\ 3 & 6 & -2 & 0 \\ 0 & 10 & -12 & 1 \\ 4 & 1 & -1 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} 4 \\ 7 \\ -1 \\ 5 \end{Bmatrix} \Rightarrow \begin{bmatrix} 4 & 1 & -1 & 1 \\ 3 & 6 & -2 & 0 \\ 0 & 10 & -12 & 1 \\ 1 & -2 & -4 & 9 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} 5 \\ 7 \\ -1 \\ 4 \end{Bmatrix}$$

- But some cannot be rearranged!

RELAXATION

$$x_i^{\text{new}} = \lambda x_i^{\text{new}} + (1-\lambda) x_i^{\text{old}}$$

- Under relaxation $(\lambda < 1)$.

$\lambda = 0.5:$

$$x_i^{\text{new}} = 0.5 x_i^{\text{new}} + 0.5 x_i^{\text{old}}$$

- Over relaxation $(\lambda > 1)$.

$\lambda = 1.5:$

$$x_i^{\text{new}} = 1.5 x_i^{\text{new}} + 0.5 x_i^{\text{old}}$$

METHODS FOR LINEAR ALGEBRAIC EQUATIONS

Method	Stability	Precision	Breadth of Application	Programming Effort	Comments
Graphical	—	Poor	Limited	—	May take more time than the numerical method but ca be useful for visualization
Cramer's rule	—	Affected by round-off error	Limited	—	Excessive computational effort required for more than three equation
Gauss elimination (with partial pivoting)	—	Affected by round-off error	General	Moderate	
LU decomposition	—	Affected by round-off error	General	Moderate	Preferred elimination method; allows computation o matrix inverse
Gauss-Seidel	May not converge if system is not diagonally dominant	Excellent	Appropriate only for diagonally dominant systems	Easy	

PROBLEMS AND REMEDIES

Method	Procedure	Potential Problems and Remedies
Gauss elimination	$\left[\begin{array}{ccc\|c} a_{11} & a_{12} & a_{13} & c_1 \\ a_{21} & a_{22} & a_{23} & c_2 \\ a_{31} & a_{32} & a_{33} & c_3 \end{array}\right] \Rightarrow \left[\begin{array}{ccc\|c} a_{11} & a_{12} & a_{13} & c_1 \\ & a'_{22} & a'_{23} & c'_2 \\ & & a''_{33} & c''_3 \end{array}\right] \Rightarrow \begin{array}{l} x_3 = c''_3/a''_{33} \\ x_2 = (c'_2 - a'_{23}x_3)/a'_{22} \\ x_1 = (c_1 - a_{12}x_1 - a_{13}x_3)/a_{11} \end{array}$	**Problems:** Ill conditioning Round-off Division by zero **Remedies:** Higher precision Partial pivoting
LU decomposition	Decomposition Back Substitution $\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \end{Bmatrix} = \begin{Bmatrix} c_1 \\ c_2 \\ c_3 \end{Bmatrix} \Rightarrow \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \end{Bmatrix} = \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix}$ Forward Substitution	**Problems:** Ill conditioning Round-off Division by zero **Remedies:** Higher precision Partial pivoting
Gauss-Seidel method	$\left.\begin{array}{l} x_1^j = (c_1 - a_{12}x_2^{j-1} - a_{13}x_3^{j-1})/a_{11} \\ x_2^j = (c_2 - a_{21}x_1^j - a_{23}x_3^{j-1})/a_{22} \\ x_3^j = (c_3 - a_{31}x_1^j - a_{32}x_2^j)/a_{33} \end{array}\right\}$ continue iteratively until $\left\| \frac{x_i^j - x_i^{j-1}}{x_i^j} \right\| 100\% < \epsilon_s$ for all x_i's	**Problems:** Divergent or converges slowly **Remedies:** Diagonal dominance Relaxation