CE4505 Surface Water Quality Engineering

Lecture 15. Numerical Methods

Numerical Methods:

Techniques by which mathematical problems are formulated so that they can be solved with arithmetic operations

Typically involve multiple, repetitive (tedious) calculations
### Numerical Techniques:

#### Examples

1. **Curve fitting (Calibration)**

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>NO3 (μg N/L)</th>
<th>Ca (mg/L)</th>
<th>error^2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>630</td>
<td>532</td>
<td>0.55</td>
</tr>
<tr>
<td>1.5</td>
<td>254</td>
<td>282</td>
<td>0.54</td>
</tr>
<tr>
<td>2.5</td>
<td>28</td>
<td>41</td>
<td>0.52</td>
</tr>
<tr>
<td>5.5</td>
<td>7</td>
<td>11</td>
<td>0.51</td>
</tr>
<tr>
<td>6.5</td>
<td>14</td>
<td>21</td>
<td>0.50</td>
</tr>
<tr>
<td>7.5</td>
<td>7</td>
<td>11</td>
<td>0.50</td>
</tr>
</tbody>
</table>

**NO3 Conc. (μg N/L)**

![Graph](image)

**SSE = 407.0666**

### Mathematical problems

<table>
<thead>
<tr>
<th>Mathematical problem</th>
<th>Numerical technique</th>
<th>Water Quality applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Roots of nonlinear equations</td>
<td>Newton-Raphson</td>
<td>Population modeling, complex kinetics</td>
</tr>
<tr>
<td>Curve fitting</td>
<td>Least-squares</td>
<td>Kinetics, Calibration</td>
</tr>
<tr>
<td>Integration – area under curves</td>
<td>Trapezoidal rule, Romberg, Gauss Quadrature</td>
<td>Water column inventories, channel sizes, River transport</td>
</tr>
<tr>
<td>Multiple linear algebraic equations</td>
<td>Gauss Elimination, Gauss-Seidel</td>
<td>Steady state multi-box models with feedback</td>
</tr>
<tr>
<td>Multiple nonlinear algebraic equations</td>
<td>Newton-Raphson Combined with Gaussian elimination</td>
<td>Equilibrium chemistry</td>
</tr>
<tr>
<td>Ordinary Differential Equations (ODEs) (Integration)</td>
<td>Euler, Heun, Runge-Kutta</td>
<td>Non-steady state single or multi-box models</td>
</tr>
<tr>
<td>Partial Differential Equations</td>
<td>Finite Element, Finite Difference</td>
<td>2-D, 3-D multi-box models (sediment porewaters, river channels, lakes, ground water)</td>
</tr>
</tbody>
</table>
Calibration: Curve fitting

\[ C = \frac{C^*}{f(\text{Cu})} \]

<table>
<thead>
<tr>
<th>Time (hr)</th>
<th>Cu Conc. (ug/L)</th>
<th>Total Cu (mole)</th>
<th>Rate (mol/L-day)</th>
<th>Avg. Cu Rate (mol/L)</th>
<th>Avg. Cu Rate (mol/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>10</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>288</td>
<td>28</td>
<td>4.4</td>
<td></td>
<td></td>
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<tr>
<td>576</td>
<td>42</td>
<td>6.6</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>1152</td>
<td>70</td>
<td>1.1</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>1728</td>
<td>100</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2304</td>
<td>124</td>
<td>1.9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2880</td>
<td>143</td>
<td>2.2</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>3456</td>
<td>160</td>
<td>2.5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4032</td>
<td>171</td>
<td>2.8</td>
<td></td>
<td></td>
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<tr>
<td>4608</td>
<td>180</td>
<td>2.8</td>
<td></td>
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</tr>
</tbody>
</table>

**SUMMARY OUTPUT**

- Multiple R: 0.9989
- R Square: 0.9977
- Adjusted R Square: 0.9974
- Standard Error: 0.0692

**ANOVA**

- df: 1, 7, 8
- SS: 14.708, 0.0335, 14.741
- MS: 14.708, 0.0048, 1.8471
- F: 3071.5, 28.10
- Significance F: 2E-10, 2E-10

**Coefficients**

- Intercept: 4.5728, 0.0425, 107.51, 2E-12
- X Variable 1: -0.495, 0.0089, -55.42, 2.8E-6

Numerical Techniques: Examples

1. Curve fitting – Least squares regression (Calibration)
Linear Regression: Least Squares

\[ A = \frac{\sum x_i^2 \sum y_i - (\sum x_i)(\sum x_i y_i)}{\Delta} \]

\[ B = \frac{N (\sum x_i y_i) - (\sum x_i)(\sum y_i)}{\Delta} \]

\[ \Delta = N \left( \sum x_i^2 \right) - \left( \sum x_i \right)^2 \]

\[ y = 4.57 - 0.50 \cdot x \]

<table>
<thead>
<tr>
<th>X values</th>
<th>Y values</th>
<th>x^2</th>
<th>x*y</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.605</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>4.127</td>
<td>1</td>
<td>4.127</td>
</tr>
<tr>
<td>2</td>
<td>3.638</td>
<td>4</td>
<td>7.276</td>
</tr>
<tr>
<td>3</td>
<td>2.996</td>
<td>9</td>
<td>8.988</td>
</tr>
<tr>
<td>4</td>
<td>2.485</td>
<td>16</td>
<td>9.94</td>
</tr>
<tr>
<td>5</td>
<td>2.079</td>
<td>25</td>
<td>10.395</td>
</tr>
<tr>
<td>6</td>
<td>1.609</td>
<td>36</td>
<td>9.654</td>
</tr>
<tr>
<td>7</td>
<td>1.099</td>
<td>49</td>
<td>7.693</td>
</tr>
<tr>
<td>8</td>
<td>0.693</td>
<td>64</td>
<td>5.544</td>
</tr>
</tbody>
</table>

\[ \sum x^2 = 23.331 \]

\[ \sum x = 4.57 \]

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>x^2</td>
<td>x*y</td>
<td>SUM</td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td></td>
</tr>
<tr>
<td>204</td>
<td>63.617</td>
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</tbody>
</table>

**Numerical Techniques: Examples**

2. Integration

![Integration Example](image)
Numerical Techniques: Examples

4. Multiple partial differential equations – Finite element/difference

Lake Superior surface temperatures

Numerical Techniques: Examples

5. Ordinary differential equations

\[ V \frac{dC}{dt} = W - \lambda C \]

\[ C = C_0 e^{-\lambda t} + \ldots \]
ODE: Crude Oiler Numerical Integrator

**Crude Euler = 1\textsuperscript{st}-order Runge-Kutta**

Projection based only on slope at current point.

\[
C_2 = C_1 + \left( \frac{dC}{dt} \right)_{t_1} \cdot \Delta t
\]

**Predicted value of** \(C_2\)

---

**ODE: 2\textsuperscript{nd}-order estimation**

**Heun’s Method = 2\textsuperscript{nd}-order Runge-Kutta**

Slope is estimated as average of initial slope and slope at predicted endpoint.

\[
C_2 = C_1 + 0.5 \cdot \left[ \left( \frac{dC}{dt} \right)_{C_1, t_1} + \left( \frac{dC}{dt} \right)_{C_2, t_2} \right] \cdot \Delta t
\]
ODE: 4th-order Runge-Kutta

\[ C_2 = C_1 + \frac{1}{6} \left[ \left( \frac{dC}{dt} \right)_{C_1,t_1} + 2 \cdot k_2 + 2 \cdot k_3 + k_4 \right] \cdot \Delta t \]

\[ k_2 = \left( \frac{dC}{dt} \right)_{C_{1+0.5\Delta t},t_{1+0.5\Delta t}} \]

\[ k_3 = \left( \frac{dC}{dt} \right)_{C_{1+0.5\Delta t},t_{2+0.5\Delta t}} \]

This is the “industry standard”

\[ k_4 = \left( \frac{dC}{dt} \right)_{C_{1+\Delta t},t_{1+\Delta t}} \]

Multiple linear algebraic equations

\[ V \frac{dx_1}{dt} = \sum W_{x_1} - (Q + k_{denitr.}V)x_1 + k_{nitrif}Vx_2 - k_{algae}Vx_3 \]
Multiple linear algebraic equations

At steady state, equations can be generalized to:

\[ C_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 \]
\[ C_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \]
\[ C_3 = a_{31}x_1 + a_{32}x_2 + a_{33}x_3 \]

To solve by hand, we would solve equation 1 for \( x_1 \) in terms of \( x_2 \) and \( x_3 \), substitute this into equations 2 and 3, rearrange the new equation 2 to solve for \( x_2 \) in terms of \( x_3 \), and substitute the expression for \( x_2 \) into equation 3, then solve equation 3 for \( x_3 \). The value for \( x_3 \) would then be substituted into equation 2 to solve for \( x_2 \), and both \( x_2 \) and \( x_3 \) would be substituted into eqn 1 which could then be solved for \( x_1 \).

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Gauss Elimination

Gauss Elimination and related methods are numerical techniques for solving multiple linear algebraic equations that also successively eliminate variables from equations and then back substitute to obtain all of the unknowns.

\[
\begin{align*}
C_1 &= a_{11}x_1 + a_{12}x_2 + a_{13}x_3 \\
C_2 &= a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \\
C_3 &= a_{31}x_1 + a_{32}x_2 + a_{33}x_3
\end{align*}
\]

\[
\begin{align*}
\text{elimination} \\
&\quad \text{elimination} \\
\text{Back substitution}
\end{align*}
\]

\[
x_1 = \frac{C_1 - \left( \frac{C_2 - \frac{C_3}{a_{33}}}{a_{22}} \right) \cdot \frac{C_3}{a_{33}}}{a_{11}}
\]

\[
x_2 = \frac{c_{22} \cdot \frac{C_2 - \frac{C_3}{a_{33}}}{a_{22}}}{a_{33}}
\]

\[
x_3 = \frac{c_{33} \cdot \frac{C_3}{a_{33}}}{a_{33}}
\]
Gauss Elimination

$C_1 = a_{11}x_1 + a_{12}x_2 + a_{13}x_3$

$C_2 = a_{21}x_1 + a_{22}x_2 + a_{23}x_3$

$C_3 = a_{31}x_1 + a_{32}x_2 + a_{33}x_3$

Step 1. Divide eqn 1 by $a_{11}$

$\frac{x_1 + \frac{a_{12}}{a_{11}}x_2 + \frac{a_{13}}{a_{11}}x_3}{a_{11}} = \frac{C_1}{a_{11}}$

Step 2. Multiply normalized equation by first coefficient of 2nd eqn.

$\frac{a_{21}x_1 + a_{21}\frac{a_{12}}{a_{11}}x_2 + a_{21}\frac{a_{13}}{a_{11}}x_3}{a_{11}} = a_{21} \frac{C_1}{a_{11}}$

Step 3. Subtract previous eqn from original eqn 2

$\left( a_{22} - a_{21}\frac{a_{12}}{a_{11}} \right)x_2 + \left( a_{23} - a_{21}\frac{a_{13}}{a_{11}} \right)x_3 = C_2 - a_{21}\frac{C_1}{a_{11}}$

Step 4. Repeat procedure to eliminate first unknown from remaining equations.
Gauss Elimination

Step 5. Repeat steps 1-4 to eliminate an additional term from each subsequent equation

\begin{align*}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= C_1 \\
a'_{22}x_2 + a'_{23}x_3 &= C'_2 \\
a''_{33}x_3 &= C''_3
\end{align*}

Step 6. Solve equation with one unknown. Substitute value for \( x_3 \) into equation with 2 unknowns; repeat back substitution until all unknowns are obtained.

Alternative methods (e.g., Gauss-Seidel) use iteration; assume a value for all but one variable, solve for the one variable and then back substitute to find other variables.