Interpolation

CHEN 1703

See also [wiki page](#) notes on interpolation.
Example - Vapor Pressure of Water

What is “vapor pressure?”

- For our purposes: the pressure at which a liquid will boil at a given temperature.
- Examples: pressure cooker, high-altitude cooking, etc.

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>P (mm Hg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.579</td>
</tr>
<tr>
<td>10</td>
<td>9.209</td>
</tr>
<tr>
<td>20</td>
<td>17.535</td>
</tr>
<tr>
<td>30</td>
<td>31.824</td>
</tr>
<tr>
<td>40</td>
<td>55.324</td>
</tr>
<tr>
<td>50</td>
<td>92.51</td>
</tr>
<tr>
<td>60</td>
<td>149.38</td>
</tr>
<tr>
<td>70</td>
<td>233.7</td>
</tr>
<tr>
<td>80</td>
<td>355.1</td>
</tr>
<tr>
<td>85</td>
<td>433.6</td>
</tr>
<tr>
<td>90</td>
<td>525.76</td>
</tr>
<tr>
<td>95</td>
<td>633.9</td>
</tr>
<tr>
<td>98</td>
<td>707.27</td>
</tr>
<tr>
<td>100</td>
<td>760</td>
</tr>
<tr>
<td>101</td>
<td>787.57</td>
</tr>
</tbody>
</table>

Determine vapor pressure of water at:
- 25 °C
- 92 °C
- 105 °C

Concept:
Fit a function to the data, and then evaluate the function wherever we need to.

Data could be from experiments, theoretical calculations, etc.
Linear Interpolation

\[ y = mx + b \]

\[ y_1 = mx_1 + b \]
\[ y_2 = mx_2 + b \]

Program this into your calculator.

\[ y = \left( \frac{y_2 - y_1}{x_2 - x_1} \right) (x - x_1) + y_1 \]

Advantages:
- Easy to use (homework, exams)
- Exact for linear functions

Disadvantages:
- Not very accurate for nonlinear functions

In MATLAB:
\[ yi=interp1(x,y,xi,\text{'linear'}) \]
- \( x \) - independent variable entries (vector)
- \( y \) - dependent variable entries (vector)
- \( xi \) - value(s) where you want to interpolate
- \( yi \) - interpolated value(s) at \( xi \).
Polynomial Interpolation

Given \( n+1 \) data points, we can fit an \( n \)-degree polynomial.

\[
p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n
\]

\[
p(x) = \sum_{i=0}^{n} a_i x^i
\]

For 4 data points, we can produce a third order polynomial to interpolate them.

\[
\begin{bmatrix}
1 & x_1 & x_1^2 & x_1^3 \\
1 & x_2 & x_2^2 & x_2^3 \\
1 & x_3 & x_3^2 & x_3^3 \\
1 & x_4 & x_4^2 & x_4^3
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2 \\
a_3
\end{bmatrix}
=
\begin{bmatrix}
y_1 \\
y_2 \\
y_3 \\
y_4
\end{bmatrix}
\]

Given \( (x_i,y_i) \), solve for \( a_i \)

Two steps:
- obtain polynomial coefficients
- evaluate the value of the polynomial at the desired location \( (x_i) \)

Example: vapor pressure data...

In MATLAB:
- \( a = \text{polyfit}(x,y,n) \)
  - requires at least \( n+1 \) points
  - if you supply more than \( n+1 \) points, then regression will be performed (more later).
- \( y_i = \text{polyval}(a,x_i) \)
  - evaluates polynomial at point(s) given by \( x_i \).
Cubic Spline Interpolation

Concept: use cubic polynomial and “hook” them together over a wide range of data...

Advantages:
• Provides a “smooth” interpolant.
• Usually more accurate than linear interpolation.
• Doesn’t get “wiggly” like higher-order polynomial interpolation can.

Disadvantages:
• Requires a bit more work than linear interpolation to implement (we won’t discuss this).

\[ yi = \text{interp1}(x, y, xi, 'spline') \]

• \( x \) - independent variable entries (vector)
• \( y \) - dependent variable entries (vector)
• \( xi \) - value(s) where you want to interpolate
• \( yi \) - interpolated value(s) at \( xi \).
If you have “structured” (tabular) data:

1. Interpolate in one direction (two 1-D interpolations)
2. Interpolate in second direction.

Use this for simple homework assignments, in-class exams, etc.

\[
\phi(x, y) \approx \frac{\phi_{1,1}}{(x_2 - x_1)(y_2 - y_1)}(x_2 - x)(y_2 - y) + \frac{\phi_{2,1}}{(x_2 - x_1)(y_2 - y_1)}(x - x_1)(y_2 - y) + \frac{\phi_{1,2}}{(x_2 - x_1)(y_2 - y_1)}(x_2 - x)(y - y_1) + \frac{\phi_{2,2}}{(x_2 - x_1)(y_2 - y_1)}(x - x_1)(y - y_1)
\]

This formula corresponds to \(x\) (first) then \(y\) interpolation

\[
\phi = \text{interp2}(x, y, \phi, x_i, y_i, 'method')
\]
- ‘linear’ - linear interpolation (default)
- ‘spline’ - spline interpolation

\(x, y\) may be vectors (matlab assumes tabular form), \(\phi\) must be a matrix.
Example - “Real” Gases

\[ p\bar{V} = zRT \]

- \( p \) - pressure
- \( z \) - compressibility factor
- \( R \) - gas constant
- \( T \) - temperature
- \( \bar{V} \) - Molar volume

\( z \) - “compressibility factor” (1 for ideal gas)

\[ \phi = \left( \frac{\phi_2 - \phi_1}{x_2 - x_1} \right) (x - x_1) + \phi_1 \]

\( \phi \) is a function of \( T \) and \( P \)

### Table

<table>
<thead>
<tr>
<th>T (K)</th>
<th>Pressure (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>300</td>
<td>0.9983</td>
</tr>
<tr>
<td>400</td>
<td>0.9995</td>
</tr>
<tr>
<td>600</td>
<td>1.0000</td>
</tr>
<tr>
<td>1000</td>
<td>1.0004</td>
</tr>
</tbody>
</table>

Source: Perry's Chemical Engineer’s Handbook (7th ed.)

MATLAB

```
interp2(x,y,\phi,xi,yi,'method')
```

Assumes that \( x \) is in columns and \( y \) is in rows of the table.

Find \( z \) at \( T=725 \) K and \( p=8 \) bar.
General 2-D Linear Interpolation

\[ \phi = ax + by + c \]

\[ \phi_1 = ax_1 + by_1 + c \]
\[ \phi_2 = ax_2 + by_2 + c \]
\[ \phi_3 = ax_3 + by_3 + c \]

\[ a = \frac{\phi_3 (y_1 - y_2) + \phi_2 (y_3 - y_1) + \phi_1 (y_2 - y_3)}{x_3 (y_1 - y_2) + x_2 (y_3 - y_1) + x_1 (y_2 - y_3)}, \]
\[ b = \frac{\phi_3 (x_2 - x_1) + \phi_2 (x_1 - x_3) + \phi_1 (x_3 - x_2)}{y_3 (x_2 - x_1) + y_2 (x_1 - x_3) + y_1 (x_3 - x_2)}, \]
\[ c = \frac{\phi_3 (x_1 y_2 - x_2 y_1) + \phi_2 (x_3 y_1 - x_1 y_3) + \phi_1 (x_2 y_3 - x_3 y_2)}{x_1 (y_2 - y_3) + x_2 (y_3 - y_1) + x_3 (y_1 - y_2)} \]

\[ \phi = \text{interp2}(x, y, \phi, xi, yi, \text{'method'}) \]

- ‘linear’ - linear interpolation
- ‘spline’ - spline interpolation

\( x, y, \phi \) are matrices (unique \( x, y \) for each \( \phi \)).