Scientific Computing
Maastricht Science Program

Week 4

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Recap

- Matlab...
- **Supervised Learning**
  - find \( f \) that maps \( \{x_1^{(j)}, \ldots, x_D^{(j)}\} \rightarrow y^{(j)} \)
  - **Interpolation**
    - \( f \) goes through the data points
  - linear regression
    - lossy fit, minimizes 'vertical' SSE
- **Unsupervised Learning**
  - PCA
  - We just have data points \( \{x_1^{(j)}, \ldots, x_D^{(j)}\} \)
Numerical Differentiation and Integration
Numerical Differentiation and Integration

- Finding derivatives or primitives of a function $f$
- not always easy or possible....
  - no closed form solution exists
  - the solution is a very complex expression that is hard to evaluate
  - we may not know $f$ (as before!)

→ numerical methods
If we want to know the rate of change...

E.g.:
- fluid in a cylinder with a hole in the bottom, measured every 5 seconds.
- High-speed camera images of animal movements, (jumping in frogs and insects, suction feeding in fish, and the strikes of mantis shrimp)
  - determine speed
  - and acceleration
Numerical Differentiation

- Determine the vertical speed at \( t = 0.25 \)

- what would you do?
Numerical Differentiation

- Determine the vertical speed at t=0.25...
  - a few options...
Numerical Differentiation

- Determine the vertical speed at \( t=0.25 \ldots \)
  - a few options...
Numerical Differentiation

- Determine the vertical speed at \( t=0.25 \ldots \)
  - a few options...

\[
\begin{array}{ccccccccccc}
0.18 & 0.2 & 0.22 & 0.24 & 0.26 & 0.28 & 0.3 & 0.32 & 0.34 & 0.36 \\
0.35 & 0.36 & 0.37 & 0.38 & 0.39 & 0.38 & 0.37 & 0.36 & 0.35 & 0.36 \\
\end{array}
\]
Numerical Differentiation

- Determine the vertical speed at t=0.25...
  - a few options...

```
<table>
<thead>
<tr>
<th>t</th>
<th>frog height(t)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.18</td>
<td></td>
</tr>
<tr>
<td>0.28</td>
<td></td>
</tr>
<tr>
<td>0.38</td>
<td></td>
</tr>
<tr>
<td>0.33</td>
<td></td>
</tr>
</tbody>
</table>

forward finite difference
backward finite difference

Other Ideas?
```
Numerical Differentiation

- Determine the vertical speed at $t=0.25$...
- a few options...

![Graph showing centered finite difference method with data points at $0.18, 0.2, 0.22, 0.24, 0.26, 0.28, 0.3, 0.32, 0.34, 0.36$]
Numerical Integration

- Integration: the reversed problem...
- Suppose we travel in a car with a broken odometer
- Speedometer is working...
Numerical Integration

- maintain speeds, to figure out traveled distance

<table>
<thead>
<tr>
<th>t</th>
<th>v(t) km/h</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>80</td>
</tr>
<tr>
<td>30</td>
<td>120</td>
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<tr>
<td>65</td>
<td>128</td>
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<tr>
<td>120</td>
<td>122</td>
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<tr>
<td>728</td>
<td>120</td>
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<tr>
<td>733</td>
<td>0</td>
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<tr>
<td>798</td>
<td>20</td>
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<td>836</td>
<td>20</td>
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<tr>
<td>941</td>
<td>70</td>
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<tr>
<td>970</td>
<td>120</td>
</tr>
<tr>
<td>1350</td>
<td>123</td>
</tr>
<tr>
<td>1404</td>
<td>90</td>
</tr>
</tbody>
</table>

- enter highway ramp
- traffic jam
- exit highway ramp
Numerical Integration

- maintain speeds, to figure out traveled distance

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Enter highway ramp

![Diagram of v(t) km/h vs time]
Numerical Integration

- maintain speeds, to figure out traveled distance

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<td>1350</td>
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How far did we travel?

enter highway ramp

exit highway ramp

traffic jam
Approximate the integral with a finite sum
Midpoint Formula

\[
\bar{x} = \frac{x_0 + x_1}{2}
\]

integration interval

\[\bar{x}_1, \bar{x}_M, H\] size of interval
Midpoint Formula

Integration interval

\[ \bar{x}_k = \frac{x_{k-1} + x_k}{2} \]

Approximation of the integral:

\[ I_{MP}(f) = H \sum_{k=1}^{M} f(\bar{x}_k) \]
Trapezoid Formula

integration interval
Trapezoid Formula

The trapezoid formula is given by:

\[ I_k = H \frac{f(x_{k-1}) + f(x_k)}{2} \]

Approximation of the integral:

\[ I_{MP}(f) = \sum_{k=1}^{M} I_k \]
Symbolic Integration

- Finally: when faced with a difficult integral...

→ try 'symbolic' packages!
Finally: when faced with a difficult integral...
→ try 'symbolic' packages!

- An easy example:
  In[48]:= f[x_] = 3*x;
  f[4]
  Out[49]= 12

  In[50]:= Integrate[f[x], x]
  Out[50]= 3*x^2/2

- A more complex example:
  In[51]:= g[x_] = Exp[x^2] * Cos[x]
     Integrate[g[x], x]
  Out[51]= e^x^2 * Cos[x]
  Out[52]= 1/4 * e^(1/4) * sqrt[pi] * (Erfi[1/2 (-i + 2 x)] + Erfi[1/2 (i + 2 x)])

- An example that has no closed form solution:
  In[53]:= h[x_] = x^3
     Integrate[h[x], x]
     N[Integrate[h[x], {x, 1, 2}]]
  Out[53]= {x^3}
  Out[54]= \{ x^3 \}
  Out[55]= \{ 13.3445 \}