WEB APP PORT OF BUFFER CAPACITY MATLAB APPLICATION

Sean Guidry Stanteen
USDA: Dr. Fred Breidt
UTA: Dr. Jianzhong Su
CONTEXT

- **pH = “potential of hydrogen”**
  - Acidity/basicity of substance
  - $\text{pH} = -\log([H^+])$, $([H^+]$ is the hydrogen ion concentration)
- **pH > 4.6 in sealed container = home for Clostridium botulinum**
  - Clostridium botulinum create toxin that causes botulism
  - Botulism = Fatal disease
HOW TO COMBAT BOTULISM?

- Make foods more acidic
  - pH < 4.6
  - $[H^+] > 10^{-4.6}$
- We don't know $[H^+]$
- But we know how to find it
HOW TO FIND \([H^+]\)

\[
0 = \sum \frac{C_{ai}K_{ai}}{K_{ai} + [H^+]} - \sum \frac{C_{bi}[H^+]}{K_{bi} + [H^+]} + \frac{K_w}{[H^+]} - [H^+] + AdjC
\]

- \(C_{a/b}\): Vector of the molar concentrations of acids and bases
- \(K_{a/b}\): Vector of corresponding equilibrium constants of acids and bases
- \(K_w = 1 \times 10^{-14}\): Autoionization constant of water
- \(AdjC\): Ion contribution due to salt in acid and bases
- Better Idea! Machine learning
  - Newton minimization
Accept parameters (.csv file)
Accept titration data from Hanna Instruments automated titrator (.RPT files)

BufferSDWebApp

BufferCapacity3
Generate buffer capacity curve via $\beta = \frac{\Delta (\text{acid or base})}{\Delta pH}$.

**BufferSDWebApp**

**BufferCapacity3**
\[ 
\min_x \sum_{i=1}^{n} (Y(pH_i) - F(pH_i; x))^2 
\]

\( Y(y) = \text{observed buffer capacity at pH } y \)

\( F(y; x) = B_0 + \sum A_i \sin \left( \frac{i}{2} y \right) + \sum B_i \cos \left( \frac{i}{2} y \right), (A_i, B_i \in x) \)

\( \beta ([H^+]; x) = 2.3 \sum_i^n \frac{C_i K_i [H^+]}{(K_i + [H^+])^2} + \frac{K_W}{[H^+]}, \text{predicted buffer capacity at } [H^+] \text{ given } x \)
## Detail Comparison

<table>
<thead>
<tr>
<th>BufferCapacity3</th>
<th>BufferSDWebApp</th>
</tr>
</thead>
<tbody>
<tr>
<td>MATLAB</td>
<td>Python, HTML, CSS, JavaScript</td>
</tr>
<tr>
<td>Desktop Application (&gt;1GB)</td>
<td>Web Application (long load time)</td>
</tr>
<tr>
<td>fmincon</td>
<td>scipy.optimize.minimize method = “trust-constr”</td>
</tr>
<tr>
<td>fminsearch</td>
<td>scipy.optimize.minimize method = “Nelder-Mead”</td>
</tr>
<tr>
<td>MATLAB App Designer</td>
<td>Flask</td>
</tr>
</tbody>
</table>
# Data Comparisons

<table>
<thead>
<tr>
<th>Ingredient (Program)</th>
<th>Anchovy MS1 (BC3)</th>
<th>Anchovy MS1 (BSD)</th>
<th>Avocado MS4 (BC3)</th>
<th>Avocado MS4 (BSD)</th>
<th>Buttermilk MS15 (BC3)</th>
<th>Buttermilk MS15 (BSD)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSE</td>
<td>2.18E-04</td>
<td>2.17E-04</td>
<td>6.96E-05</td>
<td>6.96E-05</td>
<td>9.48E-06</td>
<td>3.72E-05</td>
</tr>
<tr>
<td>Estimated pH</td>
<td>5.848</td>
<td>5.843</td>
<td>5.335</td>
<td>5.350</td>
<td>6.676</td>
<td>6.676</td>
</tr>
<tr>
<td>AdjC</td>
<td>-0.053</td>
<td>-0.053</td>
<td>-0.022</td>
<td>-0.022</td>
<td>-0.021</td>
<td>-0.022</td>
</tr>
<tr>
<td>tBeta</td>
<td>11.398</td>
<td>11.370</td>
<td>4.199</td>
<td>4.199</td>
<td>5.333</td>
<td>6.027</td>
</tr>
</tbody>
</table>

\[
MRD = \frac{1}{3} \sum_{i=1}^{3} \frac{|BC3_i - BSD_i|}{BC3_i}
\]

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<tr>
<th>SSE</th>
<th>Estimated pH</th>
<th>AdjC</th>
<th>tBeta</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9762</td>
<td>0.0012</td>
<td>0.0159</td>
<td>0.0442</td>
</tr>
</tbody>
</table>
• Companies don’t want to share their recipes
• Companies don’t want to send their recipes to other servers
• Solution: Don’t make them send it to a server
  • Pyscript: Internal Anaconda project
  • Allows Python to run client-side

INGREDIENTS: ENRICHED FLOUR (WHEAT FLOUR, NIACIN, REDUCED IRON, THIAMIN MONONITRATE [VITAMIN B₁], RIBOFLAVIN [VITAMIN B₂], FOLIC ACID), CORN SYRUP, SUGAR, SOYBEAN AND PALM OIL (WITH TBHQ FOR FRESHNESS), CORN SYRUP SOLIDS, DEXTROSE, HIGH FRUCTOSE CORN SYRUP, FRUCTOSE, GLYCERIN, CONTAINS 2% OR LESS OF COCOA (PROCESSED WITH ALKALI), POLYDEXTROSE, MODIFIED CORN STARCH, SALT, DRIED CREAM, CALCIUM CARBONATE, CORNSTARCH, LEAVENING (BAKING SODA, SODIUM ACID PYROPHOSPHATE, MONOCALCIUM PHOSPHATE, CALCIUM SULFATE), DISTILLED MONOGLYCERIDES, HYDROGENATED PALM KERNEL OIL, SODIUM STEAROYL LACTYLATED, GELATIN, COLOR ADDED, SOY LECITHIN, DATEM, NATURAL AND ARTIFICIAL FLAVOR, VANILLA EXTRACT, CARNAUBA WAX, XANTHAN GUM, VITAMIN A PALMITATE, YELLOW #5 LAKE, RED #40 LAKE, CARAMEL COLOR, NIACINAMIDE, BLUE #2 LAKE, REDUCED IRON, YELLOW #6 LAKE, PYRIDOXINE HYDROCHLORIDE (VITAMIN B₆), RIBOFLAVIN (VITAMIN B₂), THIAMIN HYDROCHLORIDE (VITAMIN B₁), CITRIC ACID, FOLIC ACID, RED #40, YELLOW #5, YELLOW #6, BLUE #2, BLUE #1.
Python functions’ inputs

Python functions’ outputs

Client Side

Server Side

Without Pyscript

Interpreter for Javascript and WebAssembly

Interpreter for Python, Java, R, etc.

Python:
\[ C = (A+B)^2 \]

Assembly:

```
MOV AX, [A] ; Move A to Register Ax
ADD AX, [B] ; Add B to A
IMUL AX ; Square(A+B)
MOV [C], AX ; Mov (A+B)^2 to C
```

Machine Code:
```
00000100 A1D01
00000103 03060F01
00000107 F7E8
00000109 A31101
0000010C C3
0000010D 0300
0000010F 0400
00000111 0000
```

Thank you StackOverflow!
With Pyscript

Client Side

Python functions and modules

Server Side

Pyodide translates functions to bytecode

Without Pyscript

Client Side

Python functions' inputs

Server Side

Python functions' outputs

Interpreter for Javascript and WebAssembly

Interpreter for Python, Java, R, etc.

Interpreter for Python functions' inputs

Python functions' outputs

Interpreter for Python functions' inputs

Python functions' outputs
SECURITY
WHAT COMES NEXT?

- Deployment on publicly available server
- Use it to produce pH estimations for multiple ingredients