Adventures with SciRuby

SciRuby Gems

- Visualization
  - rubyvis, plotrb
- Statistics
  - statsample, distribution
- Numeric
  - minimization, integration, nmatrix

https://github.com/SciRuby/nmatrix/wiki/Getting-started

NMatrix

```
>> require 'nmatrix'

>> n = NMatrix.new( [2, 4], 0)
[
 [0, 0, 0, 0]
 [0, 0, 0, 0]
]

>> NMatrix.new( 3, 0)
[
 [0, 0, 0]
 [0, 0, 0]
 [0, 0, 0]
]
```

NMatrix: Multi-Dimensional

```
>> NMatrix.new( [2, 3, 3], 0)
[
 [0, 0, 0]
 [0, 0, 0]
]

[
 [0, 0, 0]
 [0, 0, 0]
]

[
 [0, 0, 0]
 [0, 0, 0]
]
```

Simple NMatrix Constructor

```
N[ [1, 2, 3, 4] ]
=> [ [ 1, 2, 3, 4 ]]


N[ [1, 2, 3, 4], dtype: :float32 ]
=> [ [ 1.0, 2.0, 3.0, 4.0 ]]


N[ [1, 2, 3], [4, 5, 6] ]
=> [ [1, 2, 3]
     [4, 5, 6] ]
```

Rows and Columns

- Row Vector

  ```
  N[ [1, 2, 3, 4] ]
  ```

- Column Vector

  ```
  N[ [1], [2], [3], [4] ]
  N[ [1, 2, 3, 4] ].transpose
  ```

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

Element-wise Operations

```
a = NMatrix.new( [2, 2], 1)
=> [ [1, 1] [1, 1] ]

a *= 2
=> [ [2, 2] [2, 2] ]

a + a
=> [ [4, 4] [4, 4] ]

a ** 3
=> [ [8, 8] [8, 8]]
```

Dot Product

$$\begin{bmatrix} 1 & \cdot & \cdot & t_x \\ \cdot & 1 & \cdot & t_y \\ \cdot & \cdot & 1 & t_z \\ \cdot & \cdot & \cdot & 1 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix} = \begin{bmatrix} x' \\ y' \\ z' \\ 1 \end{bmatrix}$$

Dot Product

$$\begin{bmatrix} 2 & 5 & 7 \\ 6 & 10 & 3 \end{bmatrix} \cdot \begin{bmatrix} 1 & 3 \\ 6 & 5 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 46 & 38 \\ 72 & 71 \end{bmatrix}$$

$$A \cdot B \neq B \cdot A$$

$$n_{colsA} = n_{rowsB}$$

$$\begin{bmatrix} 1 & 3 \\ 6 & 5 \\ 2 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 5 & 7 \\ 6 & 10 & 3 \end{bmatrix} \quad \begin{bmatrix} 46 & 38 \\ 72 & 71 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 5 & 7 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 6 \\ 2 \end{bmatrix} = 46$$

```
a.dot(b)
=> [ [46, 38] [72, 71] ]
```

$$(2 \times 1) + (5 \times 6) + (7 \times 2) = 46$$

Ranges

```
>> NMatrix.new( [2, 5], (0..9).to_a )
[
 [0, 1, 2, 3, 4]
 [5, 6, 7, 8, 9]
]

NVector.linspace(1, 5, 5).transpose
=>
[
  [1.0, 2.0, 3.0, 4.0, 5.0]
]
```

Visualization

- plotrb
  - https://github.com/zuhao/plotrb
  - Built on Vega and D3
  - 2013 GSOC Project
  - Last commit to master about a year ago

Water/Oil Emulsion Stability with Electrolytes

$\geq$ 20 mM electrolyte:

- ▶ decreased coarsening rate
- ▶ inhibited coalescence during freeze-thaw processing
- ▶ hypothesized salt enhanced surfactant adsorption density

Aronson and Petko, *J. Colloid and Interface Sci.*,(1993), 159:134–149

Ostwald Ripening

- ≤ 12 mM
  - mean droplet size increases
  - droplet number density decreases
- 12 mM ≤ 188 mM
  - droplet size redistribution occurs
  - constant droplet number density
- > 188 mM
  - droplet size varies < 1 % over time studied

$$\pi = \frac{nRT}{V}$$

$$p_{Lp} = \frac{2\gamma}{r}$$