

Adventures with SciRuby

16 September, 2014

Michael O'Sullivan

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

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

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

$$n_{\text{rows}A} = n_{\text{cols}B}$$

$$\begin{array}{c|c} & \begin{bmatrix} 1 & 3 \\ 6 & 5 \\ 2 & 1 \end{bmatrix} \\ \hline \begin{bmatrix} 2 & 5 & 7 \\ 6 & 10 & 3 \end{bmatrix} & \begin{bmatrix} 46 & 38 \\ 72 & 71 \end{bmatrix} \end{array}$$

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

`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]  
]
```

Water/Oil Emulsion Stability with Electrolytes

≥ 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

NaCl solutions dispersed in mineral oil

Koroleva and Yurtov *Colloid Journal*, (2003), 65(1):40–43

- ▶ ≤ 12 mM
 - ▶ mean droplet size increases
 - ▶ droplet number density decreases
- ▶ $12 \text{ mM} \leq 188 \text{ mM}$
 - ▶ droplet size redistribution occurs
 - ▶ constant droplet number density
- ▶ $> 188 \text{ mM}$
 - ▶ droplet size varies $< 1 \%$ over time studied

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

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