Accelerating your Python Code For GMMs with PyCUDA

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Outline

Me = Math Major + Script Kiddy (Manage Expectations)

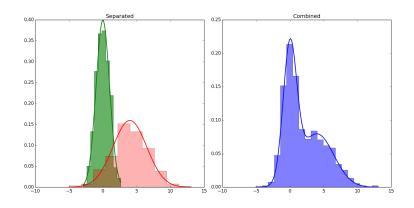
What to Expect

- Some Math
- Iterative Process I went through
- Thinking with CUDA and Basic Syntax
- How to use PyCUDA to avoid complicated work

What NOT to Expect

- How PyCUDA does it's magic
- Intermediate/Advanced CUDA

Gaussian Mixture Models d=1, K=2



K-means+=1

Gaussian Mixture Models (GMMs)

Density Function

For K mixtures

$$f(\mathbf{x}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

Log Likelihood (function of concern)

$$I(\mu, \Sigma, \mathbf{x}) = \sum_{i=1}^{N} \ln \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(x_i | \mu_k, \Sigma_k) \right)$$

Need for speed

Some post-hoc realizations

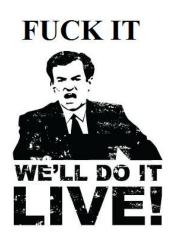
- GMM likelihood formula doesn't decompose into a mathematically simple form
- However, note that the GMM likelihood has a parallelizable form in that each point of each mixture is independent (CUDA vibes)

Computational Numbers

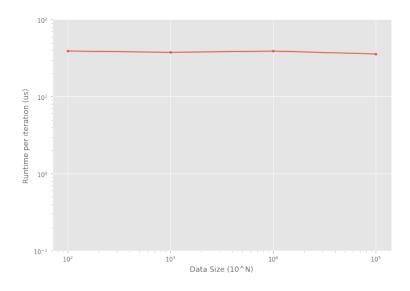
- Number of flops are of the order of O(NKd), in my case, $N=10^6$, K=8, d=13. I.e. $O(10^8)$
- I needed to evaluate the likelihood 10⁶ times for a fixed dataset while the parameters were varied. (Markov Chain Monte Carlo)
- i.e 10¹⁴ floating point operations per run.

First Attempt

- Eh, my computer is fast enough
- Pure Python (numpy)
- Took 36 us per datapoint, or 36s for whole dataset
- 10⁶ evaluations would take 1 year



Execution speed per N



Second Attempt

- Stand on the shoulders of giants (scikit-learn)
- Reverse engineered the likelihood evaluator
- 72x improvement!
- Took 0.5 us per datapoint, or 5s for whole dataset
- 10⁶ evaluations would take 5 days!



Execution speed per N

