Markov Chain Monte Carlo on the GPU

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Sampling

- Problem: given a multidimensional random variable X, want to generate samples of this random variable
- We know how to evaluate the probability density function of f_X up to a constant
- Ex: $X \sim N(\mu, \Sigma)$, an N dimensional Gaussian

$$f_X(\vec{x}) = \alpha \exp\left(-\frac{1}{2}(\vec{x}-\mu)^t \Sigma^{-1}(\vec{x}-\mu)\right)$$

- Here, $\alpha = (2\pi)^{-N/2}\det(\Sigma)^{-1/2}$. In general this normalization factor is a nuisance to compute.
- Need an algorithm to produce these samples

What is this for?

- Estimating expected values
  - Let $x_1 \dots x_K$ be samples from the distribution. Then an estimator for the expected value is given

$$E[\phi(X)] \approx \frac{1}{K} \sum_{i=1}^{K} \phi(x_i)$$

- Integrate something, usually in high dimensions
  - This can be phrased as an expected value

$$\int \phi(x) f_X(x)\, dx = E[\phi(X)] \approx \frac{1}{K} \sum_{i=1}^{K} \phi(x_i)$$

- Parameter estimation
- Simulations in statistical mechanics

Metropolis Algorithm

- The standard algorithm is the *Metropolis Algorithm*
- Design a Markov chain with relatively simple dynamics (explained shortly)
- Stationary distribution of the Markov chain is the distribution we want to sample
- Create a random walk with the Markov chain, the values of the walk are samples of the distribution
- Don't need to know the normalization factor
- This type of sampler is called a *Markov chain Monte Carlo* sampler (MCMC)

Metropolis Algorithm

- Let X_t be the sample (position of the Markov chain) at time t
- Propose a move Y by sampling from a *proposal distribution* T
  - The distribution T is something easy to sample (i.e. uniform)
  - For complicated distributions, lots of work to define a good T
- Evaluate a likelihood function for the move

$$q(Y|X_t) = \frac{T(X_t|Y)f_X(Y)}{T(Y|X_t)f_X(X_t)}$$

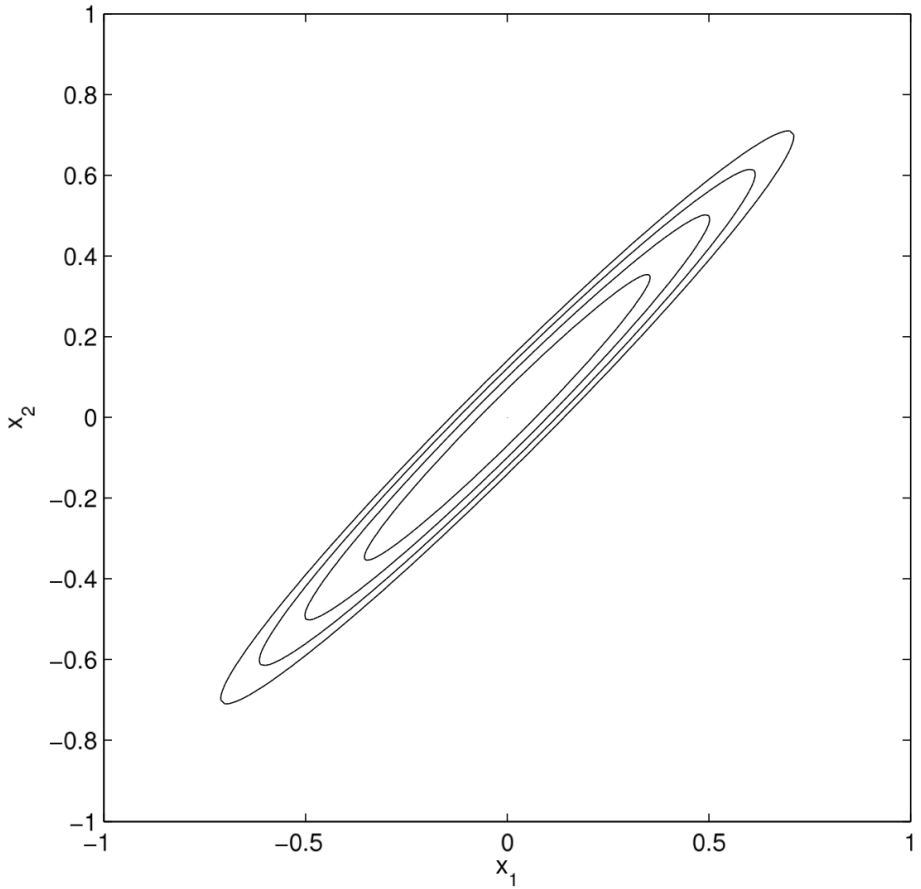
- In case of uniform T, this is $f_X(Y)/f_X(X_t)$
- If $q(Y|X_t) > 1$, accept. Otherwise, accept with probability q.
- If we accept $X_{t+1} = Y$, else $X_{t+1} = X_t$.

Problems with metropolis

- Correlation. Following samples are correlated with the previous sample.
  - Ideally samples would be independent, but the next sample is moved directly from the last
  - To quantify this, compute the *autocorrelation time* τ, a measure of the correlation of the sequence with itself.
  - If M total samples are drawn, then the effective number of independent samples is M/τ
- Serial. There is very little parallelism in this algorithm.
  - Astrophysics researchers using these methods for inference report running for days.

Skewed distributions

$$p(\vec{x}) \propto \exp\left(-\frac{(x_1 - x_2)^2}{2\epsilon} - \frac{(x_1 + x_2)^2}{2}\right)$$



Stretch Move

- Alternative MCMC method developed at Courant by Goodman and Weare in 2010
- Similar structure to Metropolis
  - Still has an accept/reject step with a likelihood calculation
- Use an *ensemble* of walkers
  - Generate a multiple samples on each iteration, each walker is a valid sample
  - Develop an update rule that allows the walkers to be updated in parallel
- Source for some figures and formulas: J. Goodman and J. Weare, *Ensemble Samplers with Affine Invariance*, Communications in Applied Mathematics and Computational Science, v. 5, 2010.

Stretch Move - Setup

- Split the walkers into two groups X_{red}, X_{black}
  - To make proofs work all cannot be updated at once
- To update a walker, randomly select a walker from the other group, then sample on a line between the two walkers.
  - This gives *affine invariance*, algorithm is not sensitive to skewed distributions
- Each group can be updated in parallel. K walkers gives precisely $K/2$ chunks of work that can be computed in parallel.
- Algorithm will require an auxiliary random variable $z \sim g(Z)$
  - Distribution must satisfy $g(1/z) = (1/z)g(z)$
  - Usually $g(z) = 1/\sqrt{2z}$ on $(1/2, 2)$
  - Picked this way to make proofs work
  - This is easy to sample by inverting CDFs. Becomes a quadratic function of a $U(0, 1)$ random variable.

Stretch Move - Algorithm

- Want to compute $X_{red}(k, t+1)$
- Randomly select a walker from the complementary ensemble $X_{black}(j)$
- Sample $z \sim g(Z)$
- Compute a proposed move Y

$$Y = X_{black}(j) + z(X_{red}(k, t) - X_{black}(j))$$

- Compute a likelihood

$$q = z^{N-1} f_X(Y) / f_X(X_{red}(k, t))$$

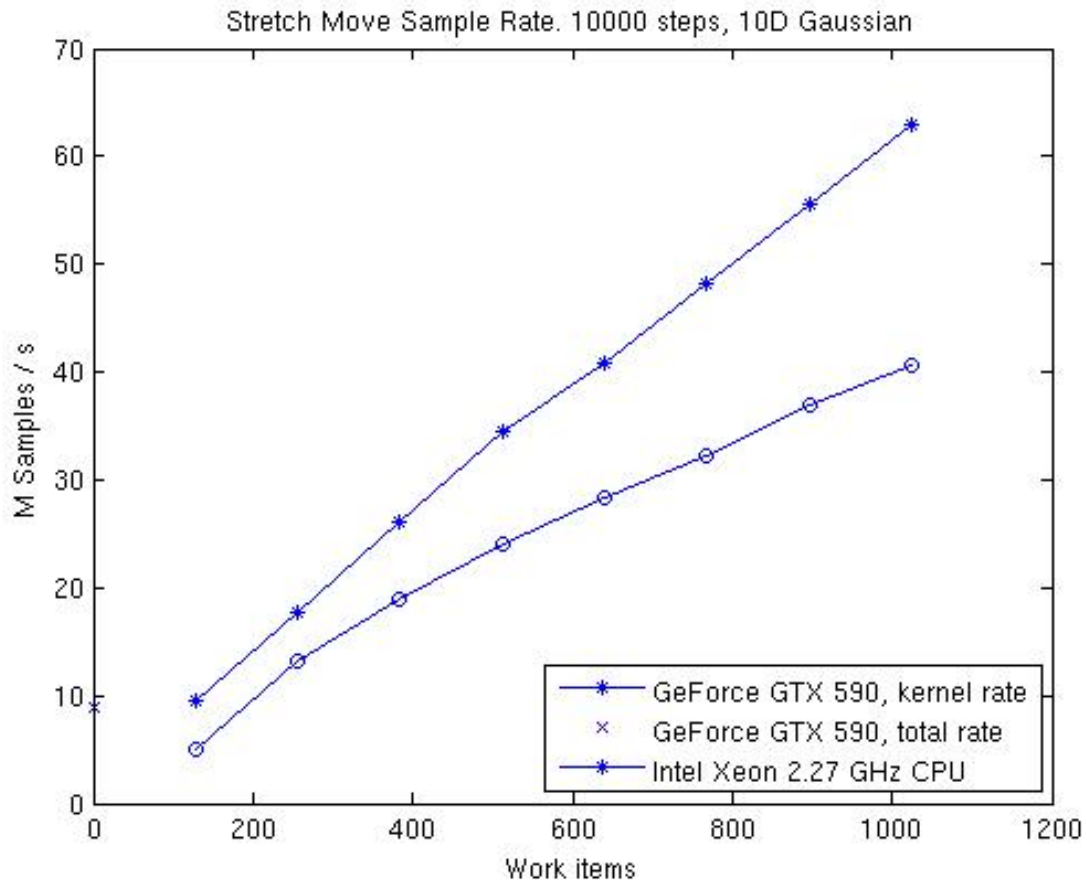
- If $q > 1$, accept. Otherwise, accept with probability q.
- If accept $X_{red}(k, t+1) = Y$, else $X_{red}(k, t+1) = X_{red}(k, t)$.

Stretch Move on the GPU

- Each work-item owns two walkers, one from each group, whole group can be updated in parallel
- Use as many walkers as can be stored in memory, up to the twice the maximum number of work-items the hardware can handle
- Barrier required before updating complementary ensemble, updated walkers need to be read
- No race conditions - clear ownership, each work-item writes to two and only two walkers
- If the PDF takes a consistent amount of time to evaluate, this is almost perfectly load balanced
- Use as many walkers as can be stored in memory, up to the twice the maximum number of work-items the hardware can handle

Stretch Move - performance

- Almost perfect linear scaling with the number of work-items.



Demo

- Looking at pre-made histograms is only so much fun. Let's make some now.

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