GPU-parallel Gibbs sampling of a hierarchical model of hybrid vigor in RNA-seq experiments

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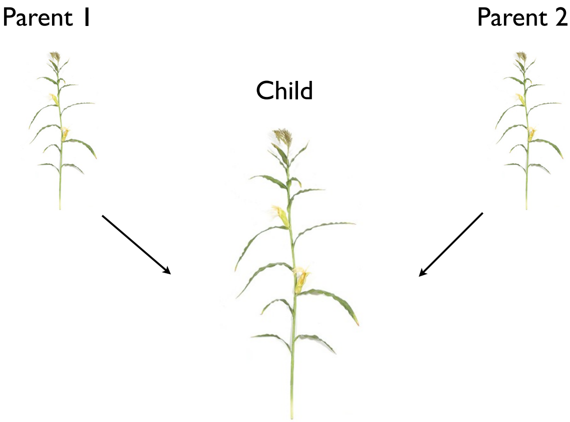
October 10, 2013

Outline

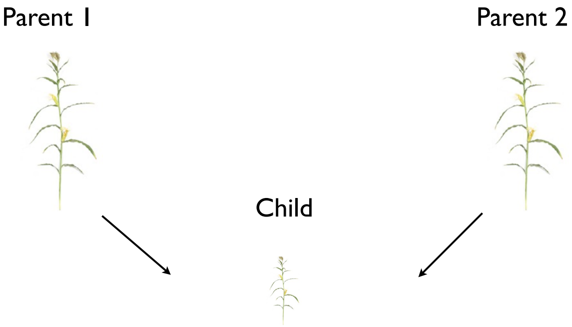
1. Biological background
   - Hybrid vigor
2. The model
3. The Gibbs sampler
   - Gibbs steps
   - Estimated heterosis probabilities
4. Acceleration with GPUs
   - An aside on GPUs
   - GPU parallelism in the model
   - Parallel reductions
5. The software

Outline

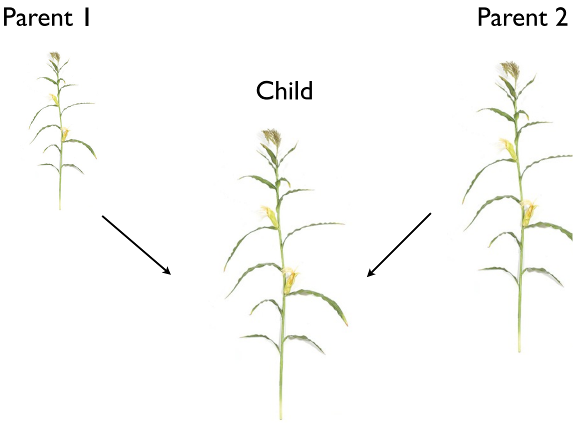
High-parent heterosis: child's trait surpasses both parents



Low-parent heterosis: child's trait is weaker than in each parent



Mid-parent heterosis: child's trait is different than average of parents



High-parent heterosis in gene expression

	Parent 1			Child		Parent 2	
Gene 1	100	225	0	70	279	300	106
Gene 2	0	1	1	50	501	2	7
Gene 3	3	4	2	700	900	0	0
Gene 4	893	400	760	5	5	1000	513
...	...	...	...	...	...	...	...
Gene 34897	10	13	6	819	761	902	912

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The model

$$\mu(g, n) = \begin{cases} \phi_g - \alpha_g & \text{sample } n \text{ from parent 1} \\ \phi_g + \delta_g & \text{sample } n \text{ from child} \\ \phi_g + \alpha_g & \text{sample } n \text{ from parent 2} \end{cases}$$

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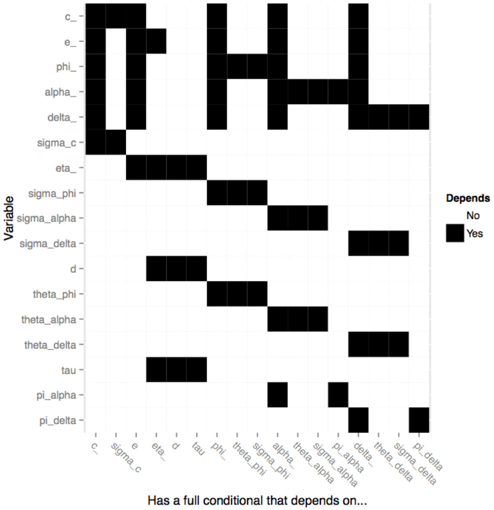
Partition parameters by conditional independence.



Use these partitions as Gibbs steps.

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- From the appropriate full conditional distributions, sample the following:

1. $c_1, \ldots, c_N$

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4. $\sigma_c, \ \sigma_\phi, \ \sigma_\alpha, \ \sigma_\delta, \ \eta_1^2, \ \ldots, \ \eta_G^2$

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5. $\varepsilon_{1,1}, \ \varepsilon_{1,2}, \ \ldots, \ \varepsilon_{1,N}, \ \varepsilon_{2,N}, \ \ldots, \ \varepsilon_{G,N}$

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5. $\varepsilon_{1,1}, \ \varepsilon_{1,2}, \ \ldots, \ \varepsilon_{1,N}, \ \varepsilon_{2,N}, \ \ldots, \ \varepsilon_{G,N}$
6. $\phi_1, \ \ldots, \ \phi_G$

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5. $\varepsilon_{1,1}, \ \varepsilon_{1,2}, \ \ldots, \ \varepsilon_{1,N}, \ \varepsilon_{2,N}, \ \ldots, \ \varepsilon_{G,N}$
6. $\phi_1, \ \ldots, \ \phi_G$
7. $\alpha_1, \ \ldots, \ \alpha_G$

Use these partitions as Gibbs steps.

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(g,n)))$$

- From the appropriate full conditional distributions, sample the following:

1. $c_1, \ldots, c_N$
2. $\tau, \pi_\alpha, \pi_\delta$
3. $d, \theta_\phi, \theta_\alpha, \theta_\delta$
4. $\sigma_c, \sigma_\phi, \sigma_\alpha, \sigma_\delta, \eta_1^2, \ldots, \eta_G^2$
5. $\varepsilon_{1,1}, \varepsilon_{1,2}, \ldots, \varepsilon_{1,N}, \varepsilon_{2,N}, \ldots, \varepsilon_{G,N}$
6. $\phi_1, \ldots, \phi_G$
7. $\alpha_1, \ldots, \alpha_G$
8. $\delta_1, \ldots, \delta_G$

- and then repeat.

Estimated heterosis probabilities

$$\mu(g, n) = \begin{cases} \phi_g - \alpha_g & \text{sample } n \text{ from parent 1} \\ \phi_g + \delta_g & \text{sample } n \text{ from child} \\ \phi_g + \alpha_g & \text{sample } n \text{ from parent 2} \end{cases}$$

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Outline

The single instruction, multiple data (SIMD) paradigm

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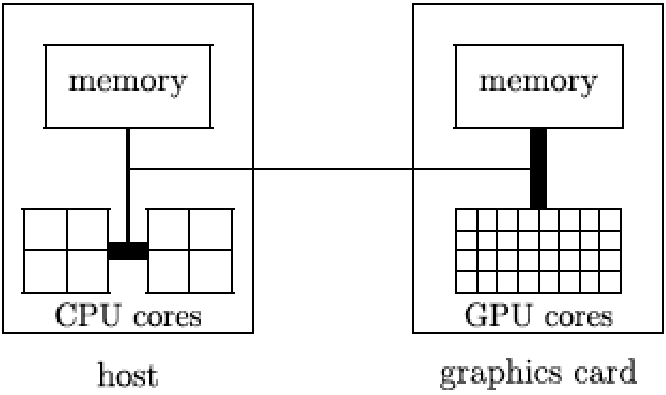
- We can similarly *parallelize* a lot more than just loops.

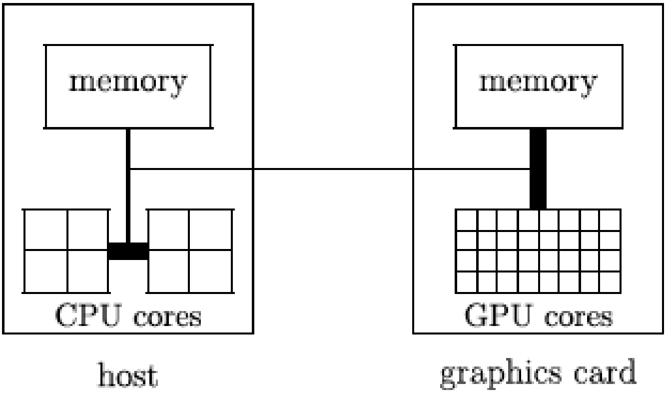
CPU / GPU cooperation

- The CPU ("host") is in charge.



CPU / GPU cooperation

- The CPU ("host") is in charge.
- The CPU sends computationally intensive instruction sets to the GPU ("device") just like a human uses a pocket calculator.



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  - CPU says: "Sum pairs of adjacent numbers. Use the array, (1, 2, 3, 4, 5, 6, 7, 8)."

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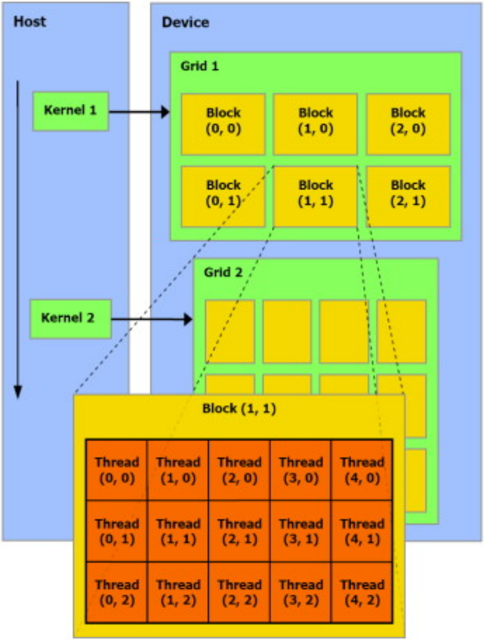
- I could have also used 1 block with 4 threads and given the threads different pairs of numbers.


Host
Device
Grid 1
Kernel 1
Block (0, 0)
Block (1, 0)
Block (2, 0)
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Block (2, 1)
Grid 2
Kernel 2
Block (1, 1)
Thread (0, 0)
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Thread (3, 0)
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Thread (3, 1)
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Tons of opportunity for GPU parallelism across genes!

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- Using parallel random walk Metropolis steps, sample the ϕ_g's from their full conditional distributions,

$$p(\phi_g \mid \cdots) \propto \exp\left(\sum_{n=1}^{N} \left[y_{g,n} \cdot \mu(g,n) - \exp(c_n + \varepsilon_{g,n} + \mu(g,n)) \right] - \frac{(\phi_g - \theta_\phi)^2}{2\sigma_\phi^2} \right)$$

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- Let's take the pairwise sum of the vector,

$$(5, 2, -3, 1, 1, 8, 2, 6)$$

using 1 block of 4 threads.

Pairwise summation: an example reduction

5 2 -3 1 1 8 2 6

6

Thread 0

Pairwise summation: an example reduction

5 2 -3 1 1 8 2 6

6 10

Thread 1

Pairwise summation: an example reduction

5 2 -3 1 1 8 2 6

6 10 -1

Thread 2

Pairwise summation: an example reduction

5 2 -3 1 1 8 2 6

6 10 -1 7

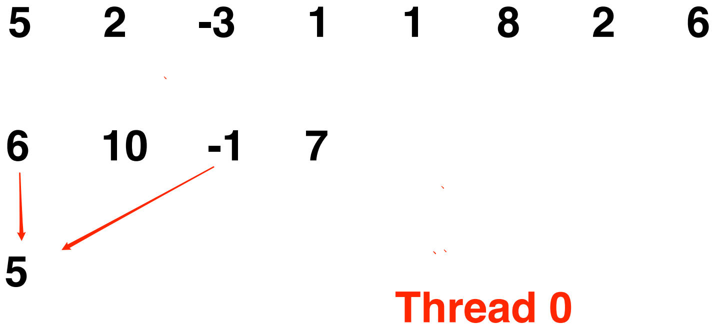
Thread 3

Pairwise summation: an example reduction

5	2	-3	1	1	8	2	6
6	10	-1	7				

Synchronize threads

Pairwise summation: an example reduction



Pairwise summation: an example reduction

5	**2**	**-3**	**1**	**1**	**8**	**2**	**6**
6	**10**	**-1**	**7**				
5	**17**						

Thread 1

Pairwise summation: an example reduction

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6	**10**	**-1**	**7**				
5	**17**						

Synchronize Threads

Pairwise summation: an example reduction

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6 10 -1 7

5 17

22

Thread 0

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- Use an efficient rejection sampler to sample τ^2.

Example: d

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- Using parallel reductions (NVIDIA's CUDA C/C++ `Thrust` library), calculate:

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- Use a random-walk metropolis step to sample d.

Outline

The software

- In progress...

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