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

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Iowa State University

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

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Biological background DNA and RNA Central dogma Examples of gene regulation RNA-seq

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Gibbs sampl Gibbs steps Estimated heterosis probabilities GPU parallelism

Outline

Biological background

DNA and RNA

Central dogma

Examples of gene regulation

RNA-sea

Hybrid vigor

The model

The Gibbs sampler

Gibbs steps

Estimated heterosis probabilities

GPU parallelism

The software

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background

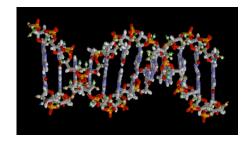
Outline

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

Biological background

DNA



··· GTGCATCTGACTCCTGAGGAGAAG ··· CACGTAGACTGAGGACTCCTCTTC ···

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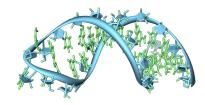
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- -

The Gibbs sample Gibbs steps Estimated heterosis

RNA



··· GUGCAUCUGACUCCUGAGGAGAAG ···

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Biological background

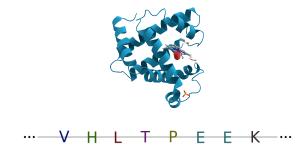
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Proteins



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DNA and RNA

Central dogma: how organisms make proteins

```
GTGCATCTGACTCCTGAGGAGAAG ...
                               DNA
```

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Central dogma

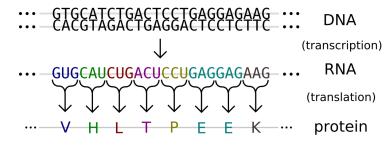
Central dogma: how organisms make proteins

GTGCATCTGACTCCTGAGGAGAAG ··· DNA (transcription) RNA GUGCAUCUGACUCCUGAGGAGAAG · · ·

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Central dogma of genetics



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Examples of gene

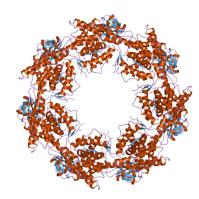
Examples of genregulation RNA-seq Hybrid vigor

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HSP₆₀

- ► HSP = heat shock protein.
- Prevent heat damage to other proteins.



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Examples of gene regulation

Temperature spike triggers HSP60 production.

HSP60 Gene

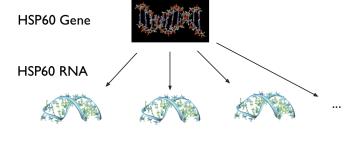


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Examples of gene regulation

Temperature spike causes HSP60 expression.



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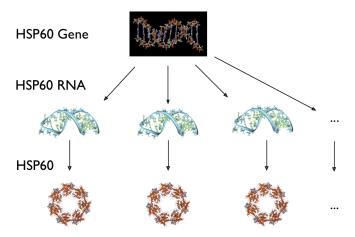
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Temperature spike causes HSP60 expression.



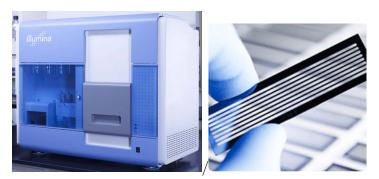
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Examples of gene regulation

RNA-seq

- RNA sequencing: measure gene expression using relative abundance of RNA.
- ► Illumina Genome Analyzer:



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RNA-seq data: counts of amplified RNA fragments

	Treatment I			Treatn	nent 2	Treatment 3	
Gene I	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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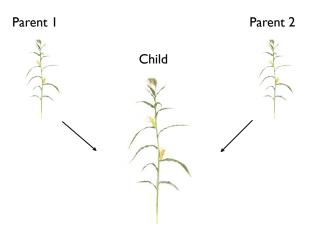
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► Goal: use RNA-seq to study hybrid vigor (heterosis).

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

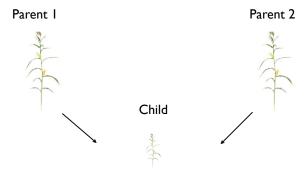


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Hybrid vigor

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



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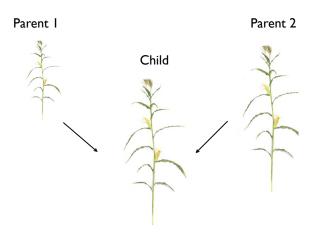
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Mid-parent heterosis: child's trait is different than average of parents



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High-parent heterosis in gene expression

	Parent I			Ch	ild	Parent 2	
Gene I	100	225	0	70	279	300	106
Gene 2	0	I	I	50	501	2	7
Gene 3	3	4	2	700	900	0	0
Gene 4	893	400	760	5	5	1000	513
	•••						
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Low-parent heterosis in gene expression

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$$\begin{aligned} y_{g,n} & \overset{\text{ind}}{\sim} \mathsf{Poisson}(y_{g,n} \mid \mathsf{exp}(c_n + \varepsilon_{g,n} + \mu(n,\phi_g,\alpha_g,\delta_g))) \\ c_n & \overset{\text{ind}}{\sim} \mathsf{N}(c_n \mid 0,\sigma_c^2) \\ & \sigma_c \sim \mathsf{U}(\sigma_c \mid 0,\sigma_{c0}) \\ \varepsilon_{g,n} & \overset{\text{ind}}{\sim} \mathsf{N}(\varepsilon_{g,n} \mid 0,\eta_g^2) \\ & \eta_g^2 & \overset{\text{ind}}{\sim} \mathsf{Inv-Gamma}\left(\eta_g^2 \mid \mathsf{shape} = \frac{d}{2} \;, \; \mathsf{rate} = \frac{d \cdot \tau^2}{2}\right) \\ & d \sim \mathsf{U}(d \mid 0,d_0) \\ & \tau^2 \sim \mathsf{Gamma}(\tau^2 \mid \mathsf{shape} = a_\tau,\mathsf{rate} = b_\tau) \end{aligned}$$

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$$\begin{split} \mu(n,\phi_g,\alpha_g,\delta_g) &= \begin{cases} \phi_g - \alpha_g & \text{sample } n \text{ from parent } 1 \\ \phi_g + \delta_g & \text{sample } n \text{ from child} \\ \phi_g + \alpha_g & \text{sample } n \text{ from parent } 3 \end{cases} \\ y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(y_{g,n} \mid \exp(c_n + \varepsilon_{g,n} + \mu(n,\phi_g,\alpha_g,\delta_g))) \\ \phi_g \overset{\text{ind}}{\sim} \text{N}(\phi_g \mid \theta_\phi, \sigma_\phi^2) \\ \theta_\phi &\sim \text{N}(\theta_\phi \mid 0, \gamma_\phi^2) \\ \sigma_\phi &\sim \text{U}(\sigma_\phi \mid 0, \sigma_{\phi 0}) \\ \alpha_g \overset{\text{ind}}{\sim} \pi_\alpha^{1-I(\alpha g)}[(1 - \pi_\alpha)\text{N}(\alpha_g \mid \theta_\alpha, \sigma_\alpha^2)]^{I(\alpha_g)} \\ \theta_\alpha &\sim \text{N}(\theta_\alpha \mid 0, \gamma_\alpha^2) \\ \sigma_\alpha &\sim \text{U}(\sigma_\alpha \mid 0, \sigma_{\alpha 0}) \\ \pi_\alpha &\sim \text{Beta}(\pi_\alpha \mid a_\alpha, b_\alpha) \\ \delta_g \overset{\text{ind}}{\sim} \pi_\delta^{1-I(\delta_g)}[(1 - \pi_\delta)\text{N}(\delta_g \mid \theta_\delta, \sigma_\delta^2)]^{I(\delta_g)} \\ \theta_\delta &\sim \text{N}(\theta_\delta \mid 0, \gamma_\delta^2) \\ \sigma_\delta &\sim \text{U}(\sigma_\delta \mid 0, \sigma_{\delta 0}) \\ \pi_\delta &\sim \text{Beta}(\pi_\delta \mid a_\delta, b_\delta) \end{split}$$

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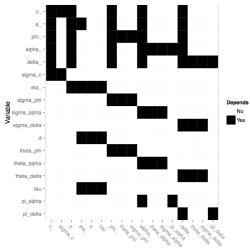
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Partition parameters by conditional independence.



Has a full conditional that depends on...

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Use these partitions as Gibbs steps.

$$y_{g,n} \stackrel{\text{ind}}{\sim} \mathsf{Poisson}(y_{g,n} \mid \exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

From the appropriate full conditional distributions, sample the following:

- 1. c_1, \ldots, c_N
- 2. τ , π_{α} , π_{δ}
- 3. d, θ_{ϕ} , θ_{α} , θ_{δ}
- 4. σ_c , σ_ϕ , σ_α , σ_δ , η_1^2 , ..., η_c^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. $\delta_1, \ldots, \delta_C$
- and then repeat.

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$$\mu(\textit{n}, \phi_{\textit{g}}, \alpha_{\textit{g}}, \delta_{\textit{g}}) = \begin{cases} \phi_{\textit{g}} - \alpha_{\textit{g}} & \text{sample } \textit{n} \text{ from parent } 1 \\ \phi_{\textit{g}} + \delta_{\textit{g}} & \text{sample } \textit{n} \text{ from child} \\ \phi_{\textit{g}} + \alpha_{\textit{g}} & \text{sample } \textit{n} \text{ from parent } 3 \end{cases}$$

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

Consider one chain with M iterations.

$$P(\text{high-parent heterosis in gene }g) pprox rac{1}{M} \sum_{i=1}^{M} I(\delta_{g}^{(i)} > |lpha_{g}^{(i)}|)$$

$$P(\text{low-parent heterosis in gene } g \) pprox rac{1}{M} \sum_{i=1}^{M} I(\delta_{g}^{(i)} < -|lpha_{g}^{(i)}|)$$

$$P(\text{mid-parent heterosis in gene } g) \approx \frac{1}{M} \sum_{i=1}^{M} I(\delta_g^{(i)} \neq 0)$$

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Biological background

Estimated heterosis probabilities

Tons of opportunity for GPU parallelism across genes!

$$y_{g,n} \stackrel{\text{ind}}{\sim} \mathsf{Poisson}(y_{g,n} \mid \exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

- Sample in parallel:
 - $\blacktriangleright \phi_g$'s
 - $ightharpoonup lpha_{
 m g}$'s
 - \triangleright δ_g 's
 - $ightharpoonup arepsilon_{{
 m g},n}$'s
 - $\rightarrow \eta_g$'s

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Example: ϕ_{σ} 's

$$y_{g,n} \stackrel{\text{ind}}{\sim} \text{Poisson}(y_{g,n} \mid \exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

$$\phi_g \stackrel{\text{ind}}{\sim} \text{N}(\phi_g \mid \theta_\phi, \sigma_\phi^2)$$

$$\theta_\phi \sim \text{N}(\theta_\phi \mid 0, \gamma_\phi^2)$$

$$\sigma_\phi \sim \text{U}(\sigma_\phi \mid 0, \sigma_{\phi 0})$$

• Using parallel random walk Metropolis steps, sample the ϕ_{σ} 's from their full conditional distributions.

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

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Tons of opportunity for GPU parallelism across genes!

$$y_{g,n} \stackrel{\text{ind}}{\sim} \text{Poisson}(y_{g,n} \mid \exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

- Use parallel reductions to calculate sufficient statistics for:
 - \triangleright C_n 'S
 - ▶ τ. d
 - \bullet θ_{ϕ} , θ_{α} , θ_{δ}
 - \triangleright σ_{ϕ} , σ_{α} , σ_{δ} , σ_{c}
 - \blacktriangleright π_{α} , π_{δ}

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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.

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Thread 0

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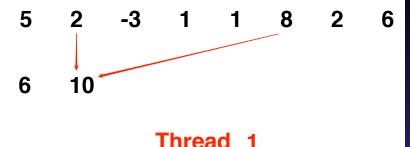
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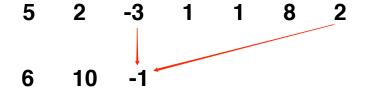
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Thread 2

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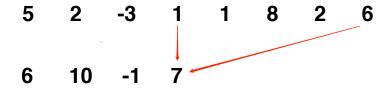
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5 2 -3 1 1 8 2 6

6 10 -1 7

Synchronize threads

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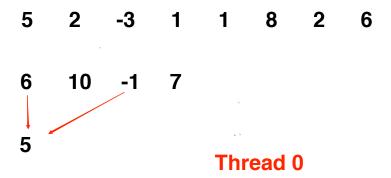
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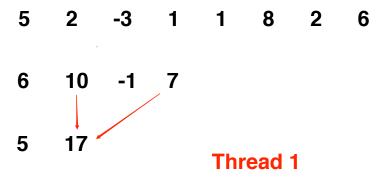
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6 10 -1 7

5 17

Synchronize Threads

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6 10 -1 7



Thread 0

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$$\begin{split} y_{g,n} & \overset{\text{ind}}{\sim} \mathsf{Poisson}(y_{g,n} \mid \mathsf{exp}(c_n + \varepsilon_{g,n} + \mu(n,\phi_g,\alpha_g,\delta_g))) \\ & \varepsilon_{g,n} \overset{\text{ind}}{\sim} \mathsf{N}(\varepsilon_{g,n} \mid 0,\eta_g^2) \\ & \eta_g^2 \overset{\text{ind}}{\sim} \mathsf{Inv-Gamma}\left(\eta_g^2 \mid \mathsf{shape} = \frac{d}{2} \;, \; \mathsf{rate} = \frac{d \cdot \tau^2}{2}\right) \\ & d \sim \mathsf{U}(d \mid 0,d_0) \\ & \tau^2 \sim \mathsf{Gamma}(\tau^2 \mid \mathsf{shape} = a_\tau,\mathsf{rate} = b_\tau) \end{split}$$

$$p(au^2 \mid \cdots)$$

$$= \mathsf{Gamma}\left(au^2 \mid \mathsf{shape} = a_{ au} + rac{\mathit{Gd}}{2} \;,\; \mathsf{rate} = b_{ au} + rac{d}{2} \sum_{g=1}^G rac{1}{\eta_g^2}
ight)$$

 Using a parallel reduction (NVIDIA's CUDA C/C++ Thrust library), calculate the sufficient statistic.

$$\sum_{g=1}^{G} \frac{1}{\eta_g^2}$$

Use an efficient rejection sampler to sample τ^2 .

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$$\begin{split} y_{g,n} &\overset{\text{ind}}{\sim} \mathsf{Poisson}(y_{g,n} \mid \exp(c_n + \varepsilon_{g,n} + \mu(n,\phi_g,\alpha_g,\delta_g))) \\ &\varepsilon_{g,n} \overset{\text{ind}}{\sim} \mathsf{N}(\varepsilon_{g,n} \mid 0,\eta_g^2) \\ &\eta_g^2 \overset{\text{ind}}{\sim} \mathsf{Inv\text{-}Gamma}\left(\eta_g^2 \mid \mathsf{shape} = \frac{d}{2} \;,\; \mathsf{rate} = \frac{d \cdot \tau^2}{2}\right) \\ &d \sim \mathsf{U}(d \mid 0,d_0) \\ &\tau^2 \sim \mathsf{Gamma}(\tau^2 \mid \mathsf{shape} = a_\tau,\mathsf{rate} = b_\tau) \\ &p(d \mid \cdots) \propto \Gamma(d/2)^{-G} \left(\frac{d \cdot \tau^2}{2}\right)^{Gd/2} \left(\prod_{g=1}^G \eta_g^2\right)^{-(d/2+1)} \exp\left(-\frac{d \cdot \tau^2}{2}\sum_{g=1}^G \frac{1}{\eta_g^2}\right) I(0 < d < d_0) \end{split}$$

▶ Using parallel reductions (NVIDIA's CUDA C/C++ Thrust library), calculate the sufficient statistics:

$$\prod_{g=1}^{G} \eta_g^2 \qquad \qquad \sum_{g=1}^{G} \frac{1}{\eta_g^2}$$

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

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► Ordinary C and GPU-accelerated versions, along with an R package wrapper, are available for download at https://github.com/wlandau/heterosis.

► Time for a demo...

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Sources

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- 7. http://en.wikipedia.org/wiki/dna
- 8. http://en.wikipedia.org/wiki/rna
- 9. http://en.wikipedia.org/wiki/HSP60

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