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Capital One

GPU Optimized Math Routines in the Stan Math Library

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MAIN GOAL

Faster model inference for Stan users ...

... in a seamless and cost-effective way.

TALK OUTLINE

- Motivation: GP regression.
- Parallelization & GPUs.
- Stan + OpenCL.
- Paralellizing the Cholesky decomposition.
- Challenges & Roadmap.

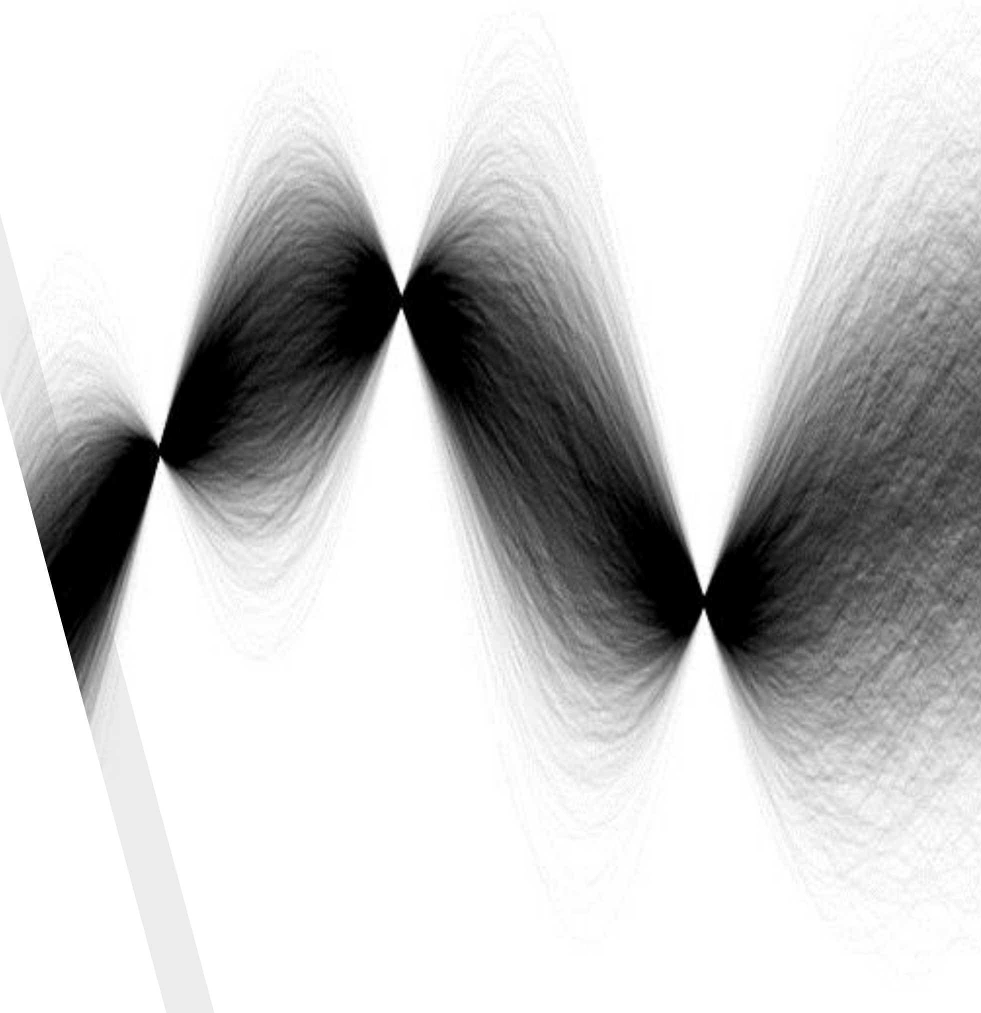
GP REGRESSION

Gaussian Processes are very useful but ...

... computation scales unfavorably - $O(n^3)$.

What can we do?

- Approximate inference.
- Run the computation on a better CPU.
- Run the computation in parallel.



PARALLELIZATION 101

Break the problem up into smaller pieces and compute them in parallel.

The pieces must be:

- Small enough to keep all individual processing units busy most of the time.
- Large enough to avoid too much overhead with breaking them up and putting them back together.

Maximum speedup limited by the parts we can‘t parallelize.

WHY GPUs?

Properties of GPUs:

- Everyone has a GPU.
- Massive parallelism – thousands of „cores“ (best performance/cost ratio).
- Optimized for vector and matrix problems.
- Faster data transfers compared to clusters.
- Energy efficient.

Stan
+ OpenCL

OpenCL

- Parallel framework CPUs, GPUs, DSPs, FPGAs,...
- Special functions (kernels) are executed by N threads on target devices.
- APIs for C, C++, Python, Julia...
- Open standard maintained by the Khronos Group.

Typical example:

- Copy input data to the OpenCL device,
- parallel execution of special functions on the OpenCL device and
- copy the results back to the host.

What‘s an OpenCL **Context**?

It‘s like a scheduler:

- Manages the devices, queues, platforms, memory alloc, etc.
- Devices: GPUs and CPUs.
- Platforms: Implementations of OpenCL (Khronos’s OpenCL vs. Intel’s OpenCL).
- The context has a ‘program’ object that manages kernels for devices and platforms.

OpenCL **Context**

- We only want one context to exist so it's stored as a singleton.
- Access the context through an adapter API.

IE: In the adapter class `opencl_context`

```
// Return the stan program's context
inline cl::Context& context() {
  return opencl_context_base::getInstance().context_;
}

...

// developers access
auto ctx = opencl_context.context()
```

Mimic Vat 3

Artifact

Imprint — Whenever a nontoken creature is put into a graveyard from the battlefield, you may exile that card. If you do, return each other card exiled with Mimic Vat to its owner's graveyard.

3, ↷: Put a token onto the battlefield that's a copy of the exiled card. It gains haste. Exile it at the beginning of the next end step.

Matt Cavotta

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Making Kernels

- We want to make it simple for users to add and use kernels.
- Reworked design with Sean Talts and Rok.

Making a kernel:

A kernel that only needs to set the global work size.

Name of kernel

```
const global_range_kernel<cl::Buffer, cl::Buffer, int, int> copy("copy", copy_kernel_code);
```

Argument Types kernel accepts

String literal holding the kernel code

Accessing Matrices
on the Device

Developers move Stan matrices over to `matrix_cl` matrices:

```
matrix_d d1
matrix_cl d1_cl(d1)
```

Users operate on these like Stan matrices:

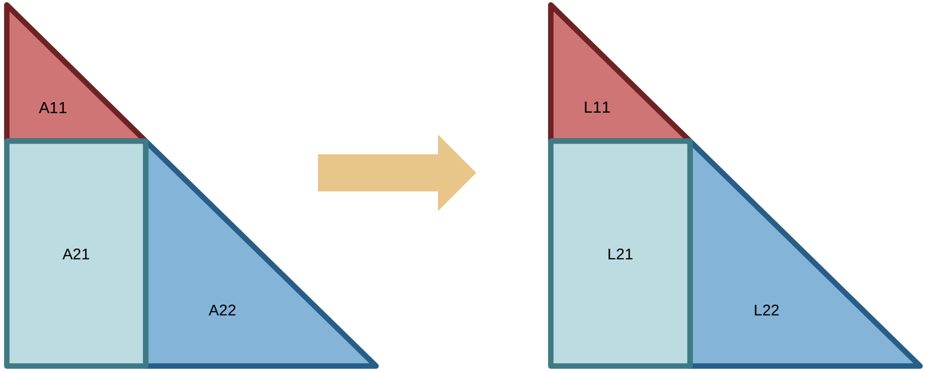
```
matrix_cl d3_cl = d1_cl + d2_cl
matrix_cl d4_cl = cholesky_decompose(d1_cl)
```

OpenCL

First GPU-optimization available to Stan users:

Cholesky Decomposition

Cholesky Decomposition



- Our first bottleneck target in Stan.
- Almost no naive parallelims in the basic algorithm.
- No real speedup on the GPU.
- Blocked-cholesky is computationally more complex but GPUs are made for fast matrix multiplications.

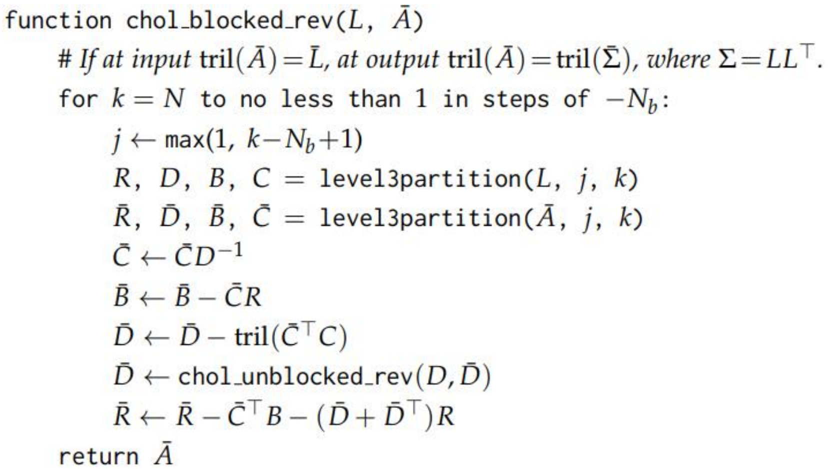
Derivative of the Cholesky Decomposition

GPU implementation of [Murray 2016]:

- Eigen version already in Stan Math,
- largest bottlenecks are matrix multiplication and lower triangular inverse.

As a consequence - GPU implementations of

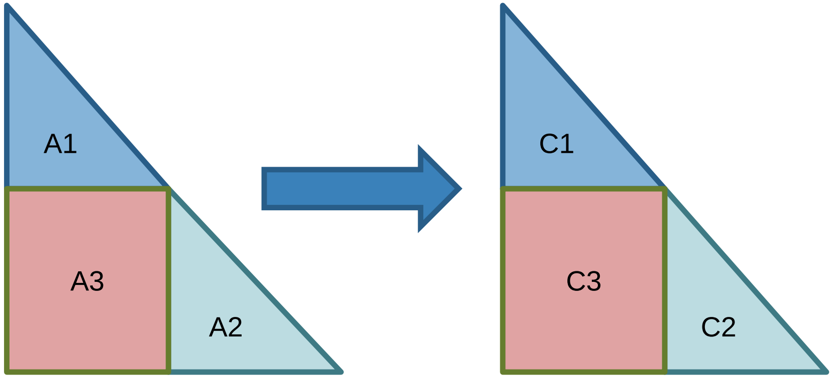
- matrix multiplication,
- lower triangular inverse,
- +, -, transpose, partition.



```
function chol_blocked_rev($L$, $\bar{A}$)
    # If at input $\mathrm{tril}(\bar{A}) = \bar{L}$, at output $\mathrm{tril}(\bar{A}) = \mathrm{tril}(\bar{\Sigma})$, where $\Sigma = LL^\top$.
    for $k = N$ to no less than 1 in steps of $-N_b$:
        $j \leftarrow \max(1,\ k - N_b + 1)$
        $R,\ D,\ B,\ C$ = level3partition($L$, $j$, $k$)
        $\bar{R},\ \bar{D},\ \bar{B},\ \bar{C}$ = level3partition($\bar{A}$, $j$, $k$)
        $\bar{C} \leftarrow \bar{C}D^{-1}$
        $\bar{B} \leftarrow \bar{B} - \bar{C}R$
        $\bar{D} \leftarrow \bar{D} - \mathrm{tril}(\bar{C}^\top C)$
        $\bar{D} \leftarrow$ chol_unblocked_rev$(D, \bar{D})$
        $\bar{R} \leftarrow \bar{R} - \bar{C}^\top B - (\bar{D} + \bar{D}^\top)R$
    return $\bar{A}$
```

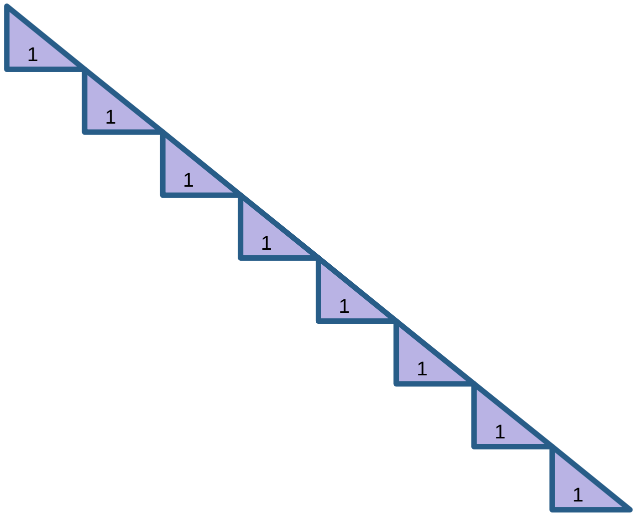
Lower triangular inverse

GPU Basic forward substiution algorithm not suitable for GPUs.

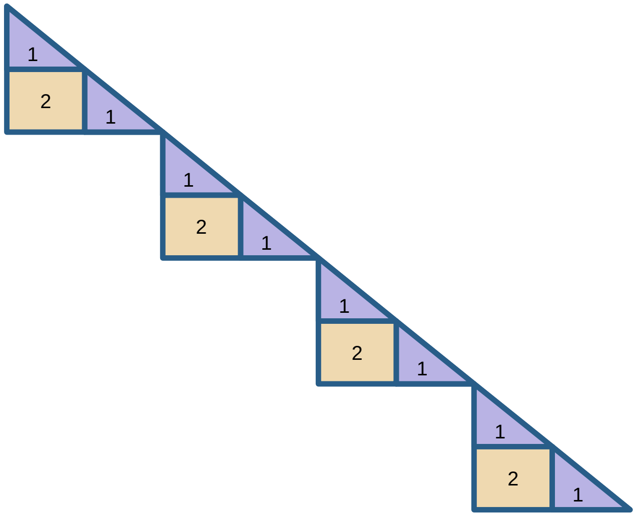


$$C_1 = A_1^{-1}$$
$$C_2 = A_2^{-1}$$
$$C_3 = -C_2 A_3 C_1$$

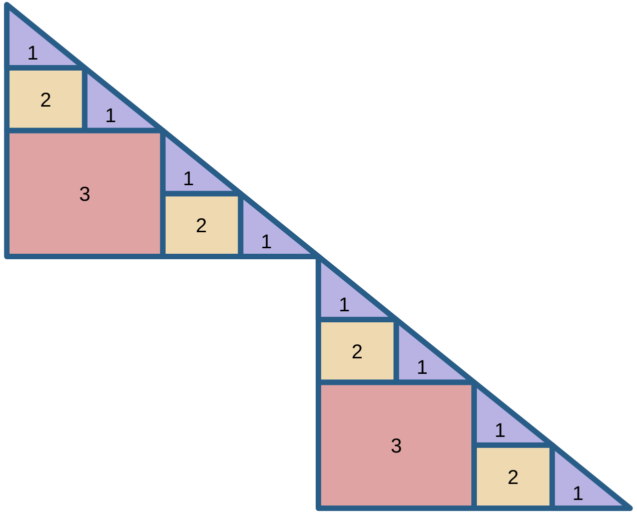
Lower triangular inverse



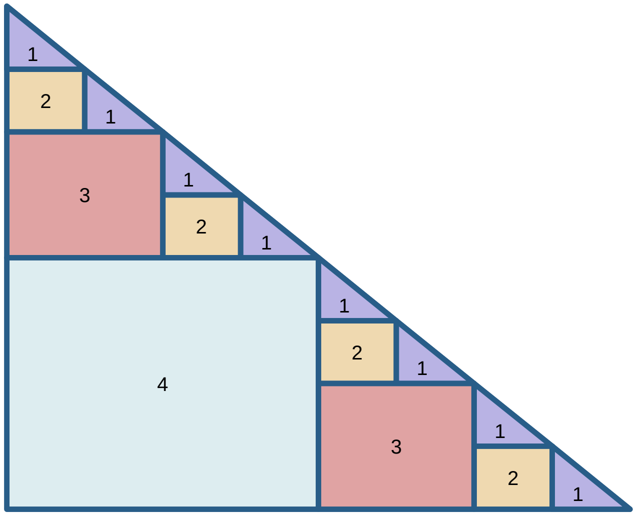
Lower triangular inverse



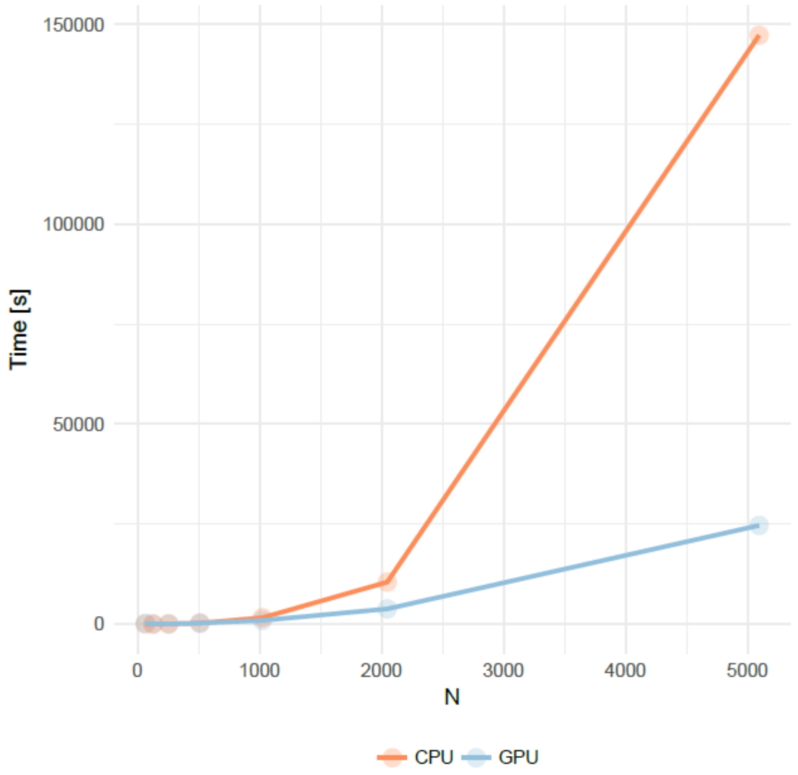
Lower triangular inverse

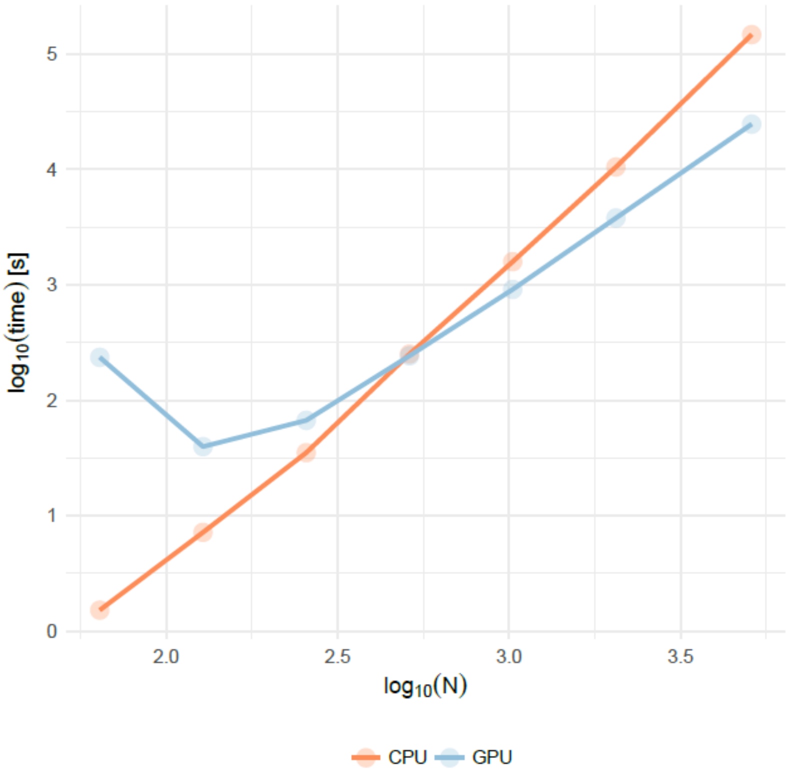


Lower triangular inverse

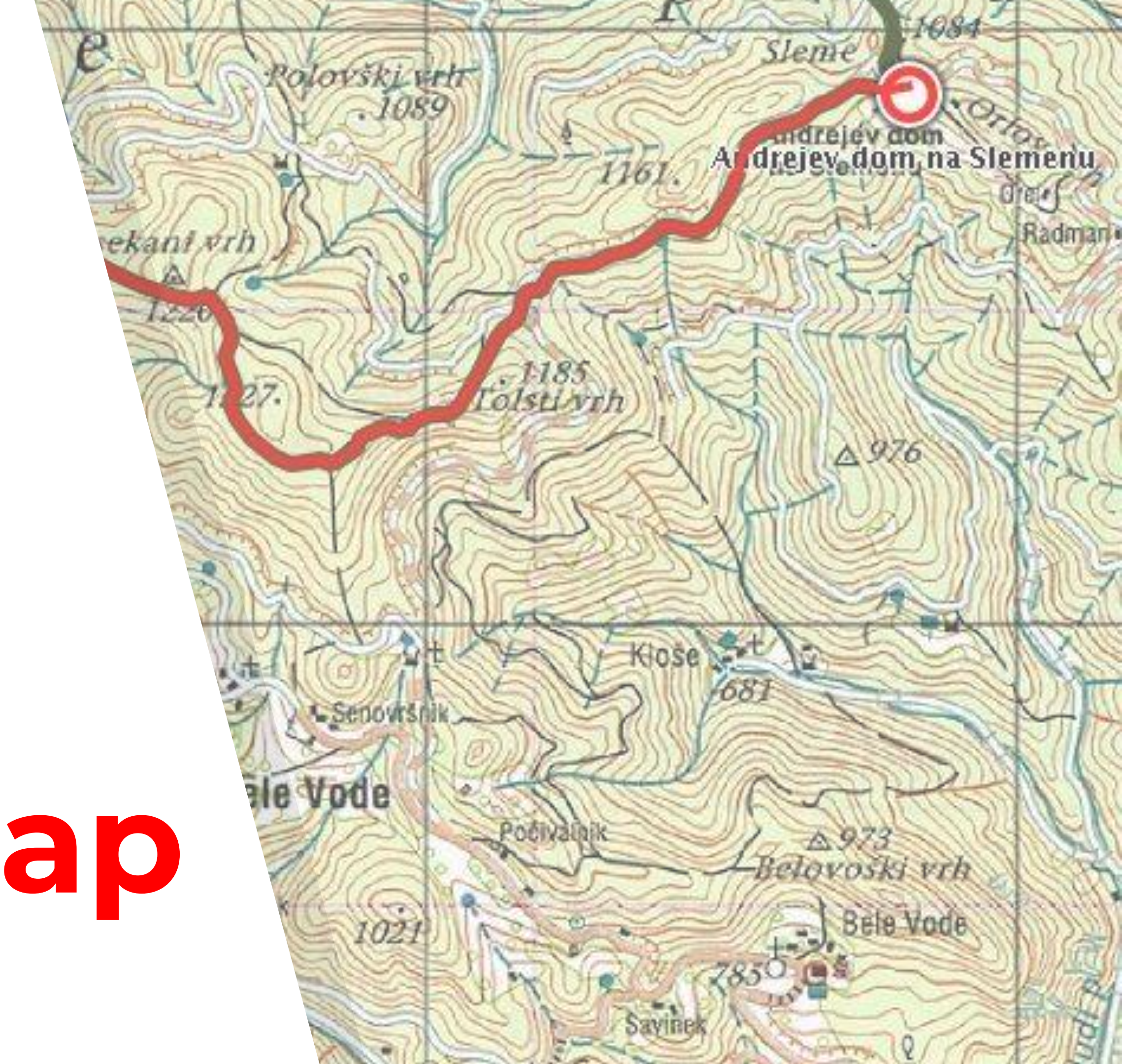


RESULTS (simple 1D GP regression on N points)





Issues & Roadmap



Issue: Data tranfers

Currently, speedups are limited by data transfers:

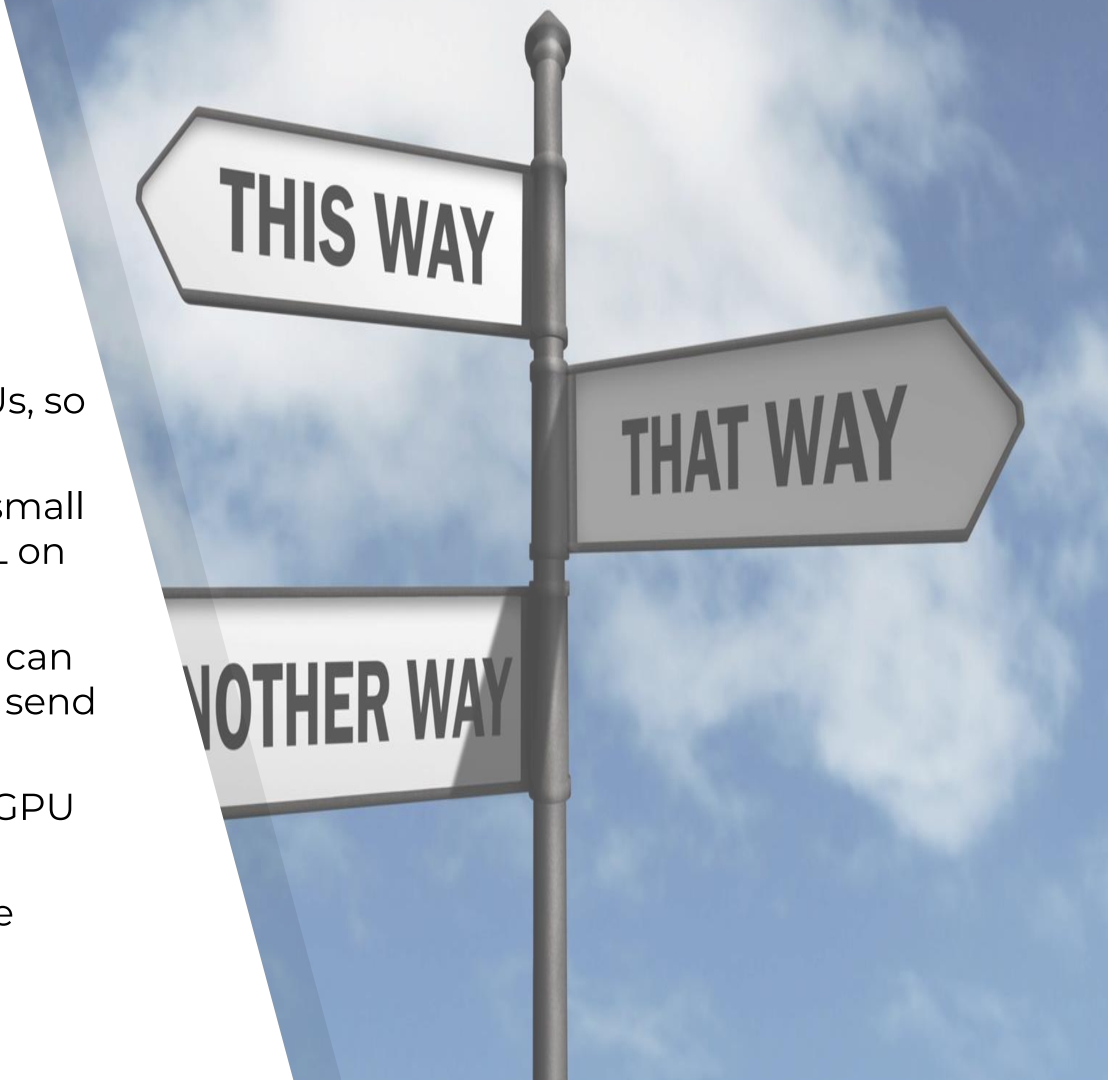
- Copying data to the GPU costs us some time.
- Most functions scale linearly and can‘t justify this cost for every call.
- Even is such functions represent 10% of the computation, it drastically limits the maximum speedup.

Example:

```
cov_exp_quad(x1, magnitude_1, length_scale_1)
  + cov_exp_quad(x1, magnitude_2, length_scale_2)
  + gp_periodic_cov(x1, magnitude_3, length_scale_3_1, 7)
 .* cov_exp_quad(x1, 1.0, length_scale_3_2)
  + gp_periodic_cov(x1, magnitude_4, length_scale_4_1, 365.25)
 .* cov_exp_quad(x1, 1.0, length_scale_4_2)
  + gp_dot_prod_cov(I_s, magnitude_5_1)
  + gp_dot_prod_cov(I_ss, magnitude_5_2)
  + gp_dot_prod_cov(I_ws, magnitude_5_3)
  + diag_matrix(rep_vector(jitter, N2));`
```

Multiple Devices and OOM Algorithms

- OpenCL can run on CPUs and GPUs, so why not use both?
- We know some problems are too small to send to the GPU, so use OpenCL on the CPU.
- Needs a ‘smart’ load balancer that can look at a ‘job’ and decide where to send it.
- Current algorithms are limited by GPU DRAM.
- We should be able to configure the algorithms to work in a chunking fashion.



From single routines to (almost) entire models

Idea: move the bulk of the log-posterior computation (including „hand-made“ gradients) to the GPU.

Promising results on some models (~100x speedup).

Currently in the works:

- GLM (linear, logistic, Poisson, NB regression...). For example:

  ```
  bernoulli_logit_glm_lpdf(y | X, beta, alpha);
  ```

- Roadblock: Data transfers!