GPU Optimized Math Routines in the Stan Math Library

Rok Češnovar, Davor Sluga, Jure Demšar, Steve Bronder, Erik Štrumbelj

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.

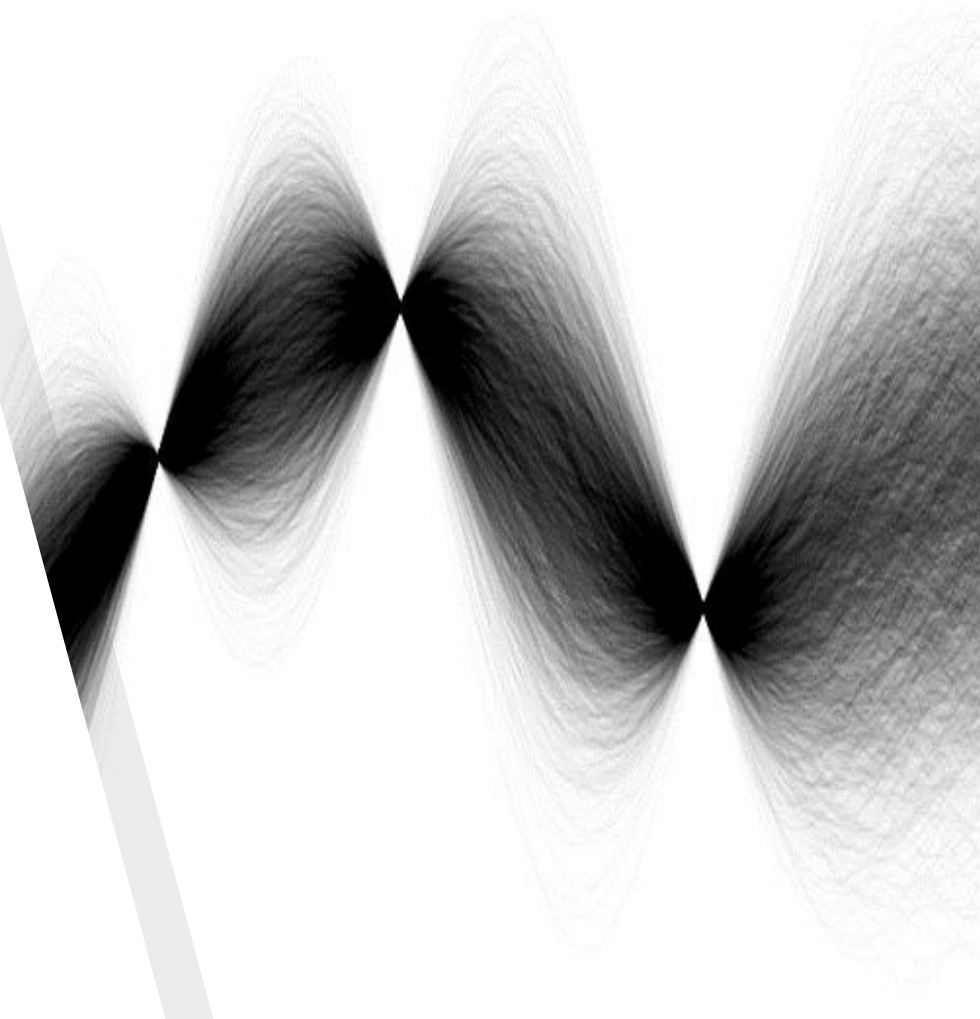
GP REGRESSION

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 (thanks, Amdahl!).

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()
```

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)
```

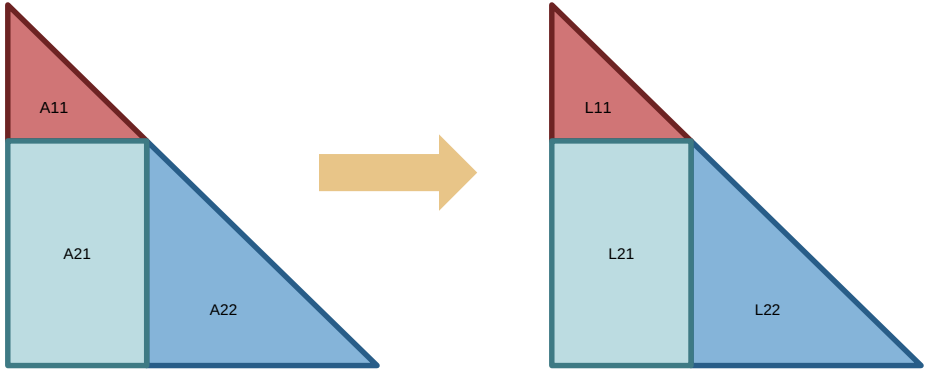
Users operate on these like Stan matrices:

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

First GPU-optimization available to Stan users:

Cholesky Decomposition

Cholesky
Decomposition



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

$$L_{21} = A_{21}(L_{11}^{T})^{-1}$$
$$L_{22} = A_{22} - L_{21}(L_{21})^{T}$$

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.

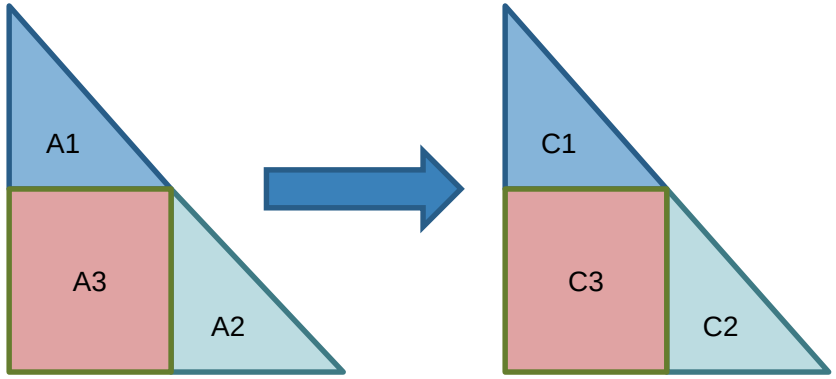
As a consequence - GPU implementations of

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

```
function chol_blocked_rev(L, Ā)
    # At input tril(Ā) = L̄, at output tril(Ā) = tril(Σ̄), where Σ = LL^⊤.
    for k = N to no less than 1 in steps of −N_b:
        j ← max(1, k − N_b + 1)
        R, D, B, C = level3partition(L, j, k)
        R̄, D̄, B̄, C̄ = level3partition(Ā, j, k)
        C̄ ← C̄D^{−1}
        B̄ ← B̄ − C̄R
        D̄ ← D̄ − tril(C̄^⊤C)
        D̄ ← chol_unblocked_rev(D, D̄)
        R̄ ← R̄ − C̄^⊤B − (D̄ + D̄^⊤)R
    return Ā
```

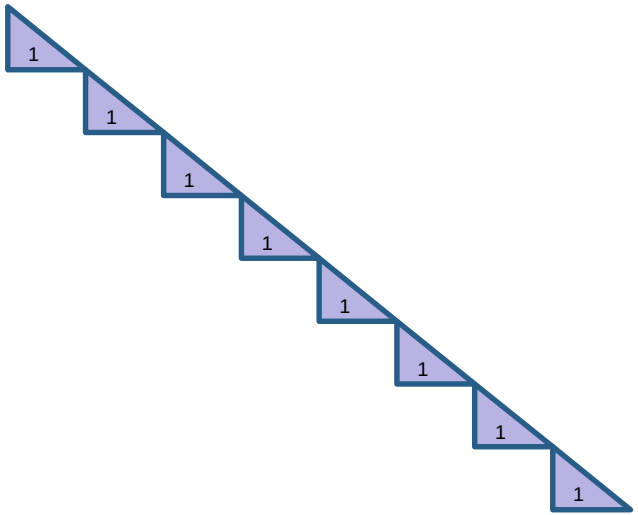
Lower triangular inverse

GPU Basic forward substiution algorithm not suitable for GPUs.

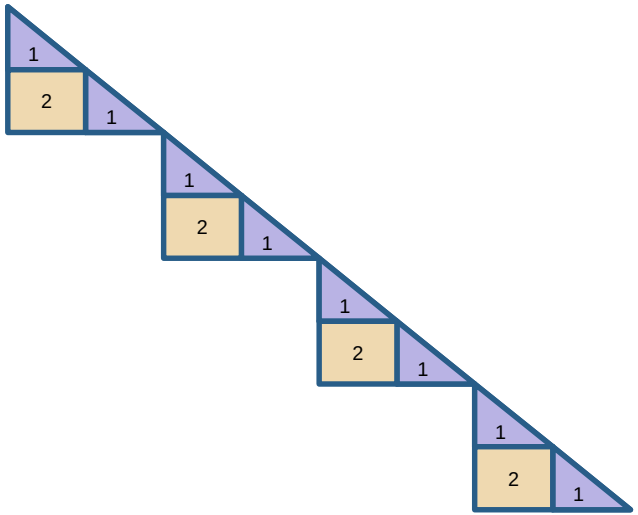


$$C_1 = A_1^{-1}$$
$$C_2 = A_2^{-1}$$
$$C_3 = -C_2 A_3 C_1$$

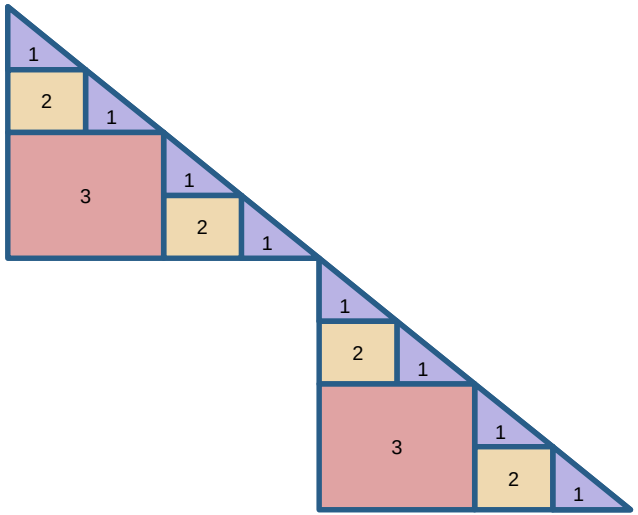
Lower triangular inverse



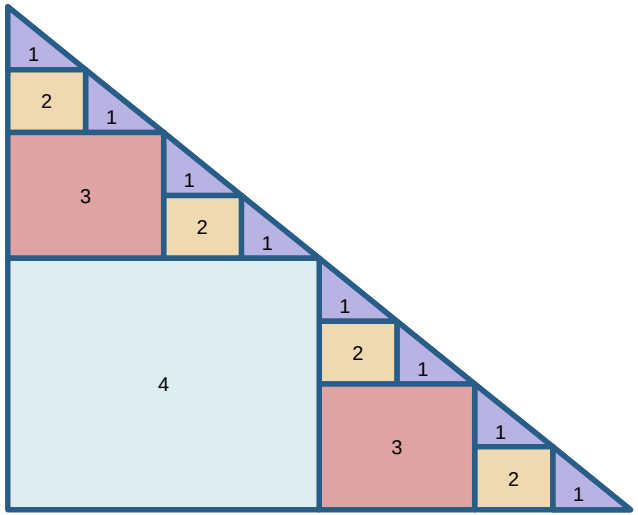
Lower triangular inverse



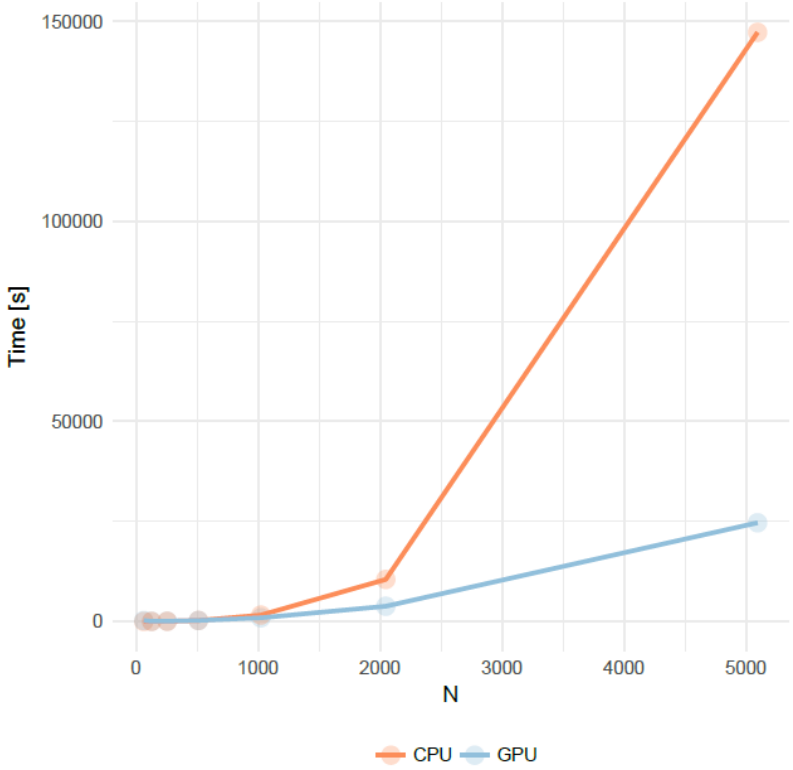
Lower triangular inverse

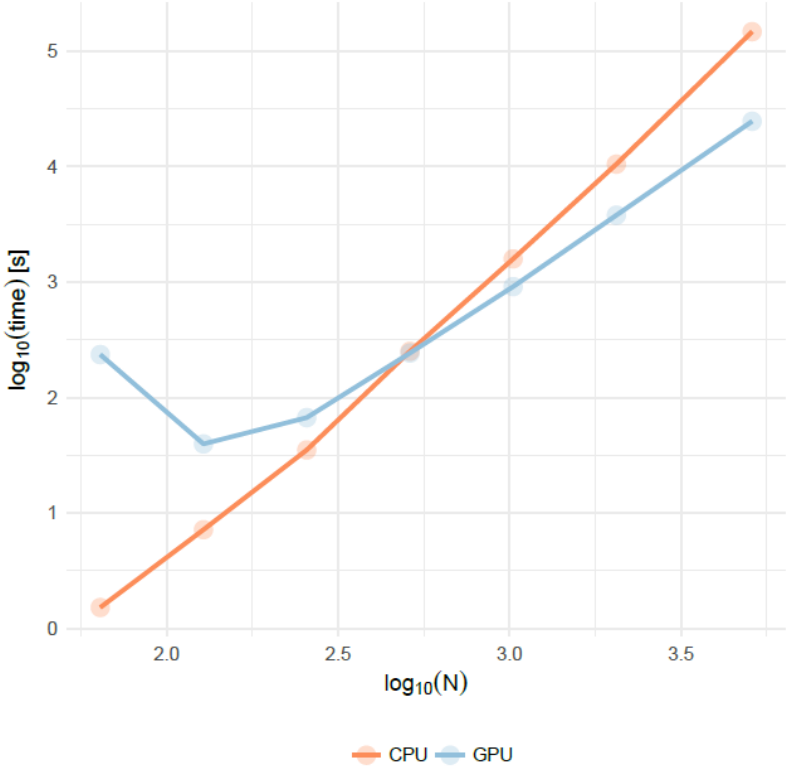


Lower triangular inverse

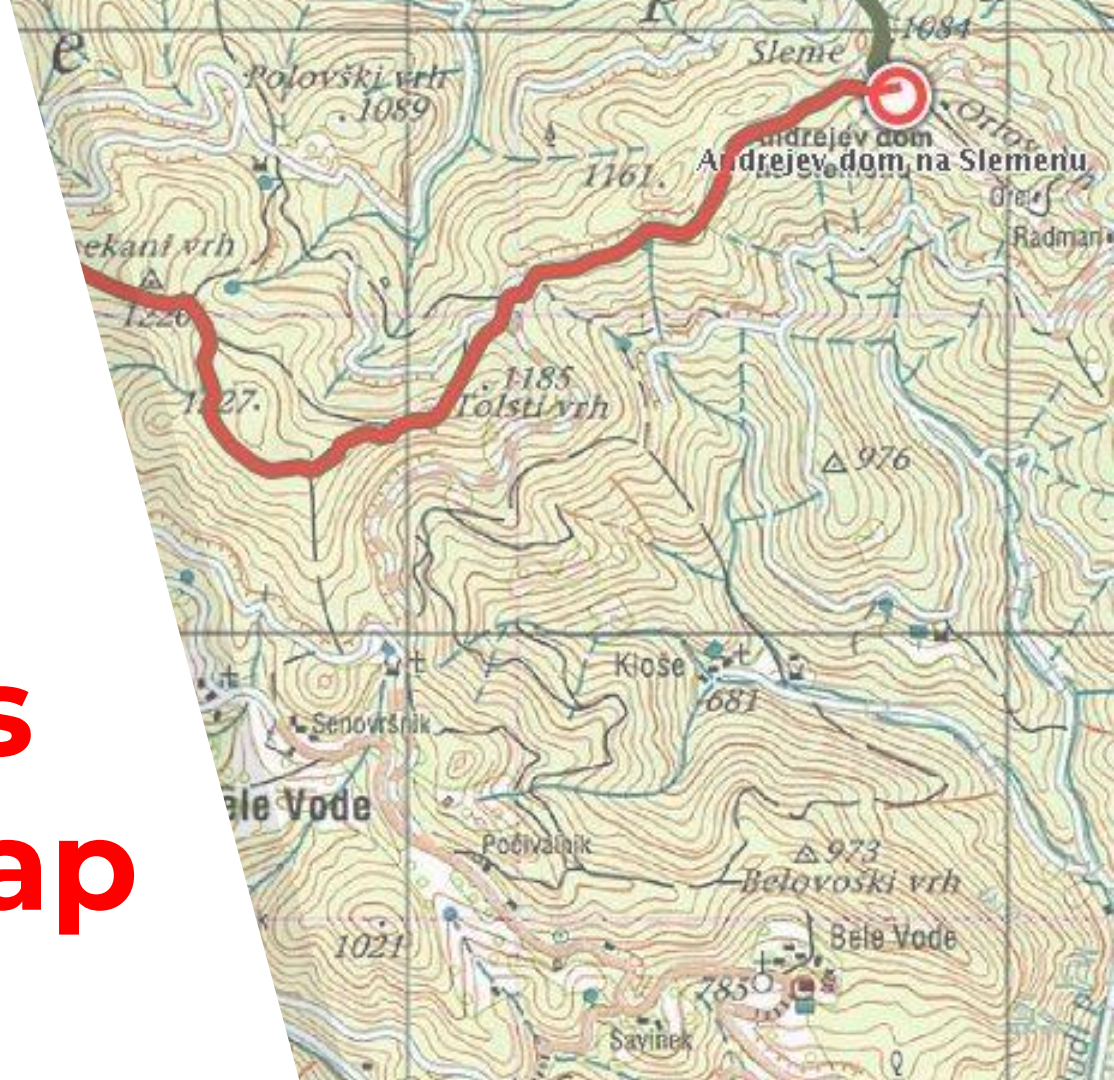


RESULTS (simple 1D GP regression on N points)





Challenges & Roadmap



Issue: Data tranfers

Currently, speedups are limited by data transfers:

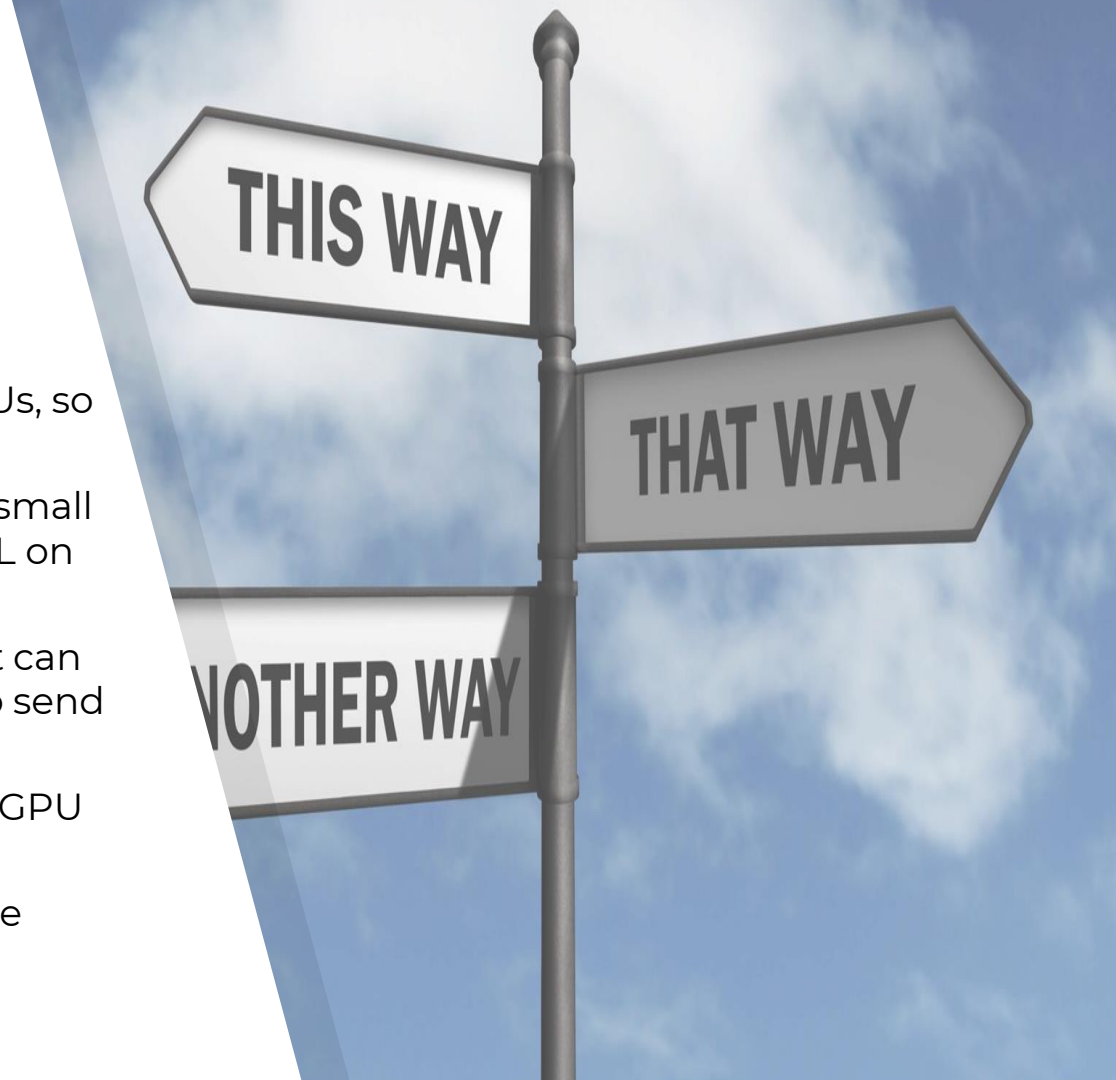
- Copying data to the GPU costs us some time.
- Most functions scale linearly and can‘t justify this cost for every call.
- Even is such functions represent 10% of the computation, it drastically limits the maximum speedup.

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!

Conclusion

- GPU support in Stan: Coming very soon!
- First, inverting covariance matrices...
- ... other building-blocks will follow.
- Reasonable expectation: 10-200x speedup

.

If you have any questions, comments, ideas... let us know! We‘re also accepting requests. ☺