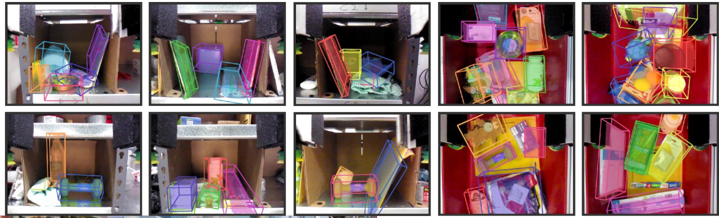
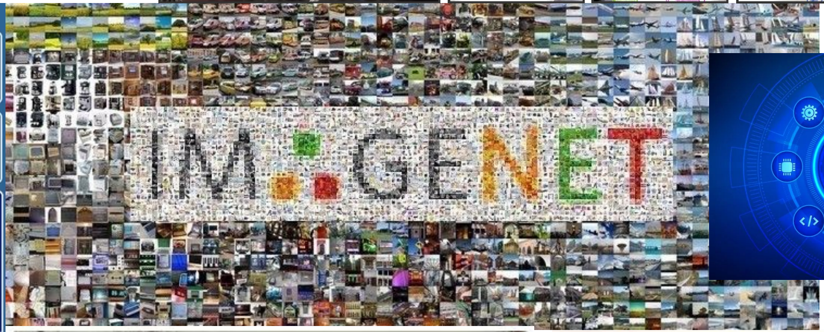
Accelerating Graph Convolutions

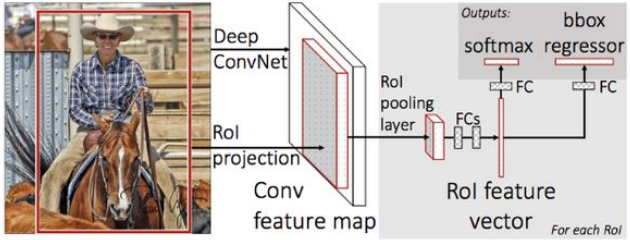
A Simple Python Runtime System Built for CS263

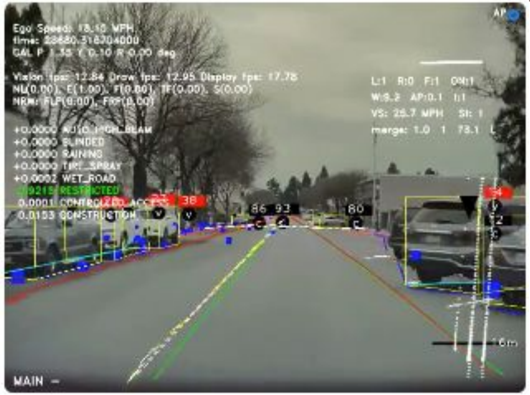
Yuke Wang and Sirius Zhang

So Called AI Revolution









Our Project / Presentation Milestones

- Looked at runtime system’s role in this “AI” revolution.
- Implemented a runtime system for Graph Convolutional Networks (GCN)
- Profiled performance difference and runtime bottleneck.

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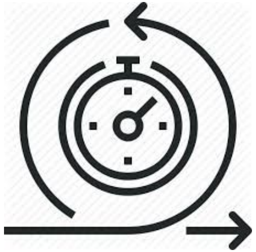
What Data Scientists / ML Researchers Need?

- Fast iteration in algorithm development.
- Matrix, tensor (“matrix” > 2D), and linear algebra are the workhorse of all math-heavy, data-hungry algorithms.
- Fast matrix / tensor calculation, potentially accelerated through parallel computing hardware.

$$\begin{bmatrix} a_1 & a_2 & a_3 \\ a_4 & a_5 & a_6 \\ a_7 & a_8 & a_9 \end{bmatrix} \begin{bmatrix} b_1 & b_2 & b_3 \\ b_4 & b_5 & b_6 \\ b_7 & b_8 & b_9 \end{bmatrix} = \begin{bmatrix} c_1 & c_2 & c_3 \\ c_4 & c_5 & c_6 \\ c_7 & c_8 & c_9 \end{bmatrix}$$

NVIDIA



How Runtime System Helped in this Revolution?

- Use High level language such as Python to cover up low-level machine programming details.
- For performance, bringing in CUDA and C/C++, and use them under the hood for performance critical places.

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- Looked at runtime system's role in this "AI" revolution.
- Implemented a runtime system for Graph Convolutional Networks (GCN).
    - Overall Goal
    - Intro to GCN
    - Implemented two variants of Graph convolutional kernels used a mixed of CUDA/C++/Python code.
        - Scatter & Gather (SAG) kernel
        - Sparse Matrix and Matrix Multiplication (SpMM) kernel
    - Python Wrapper
        - Different Variants
        - Our Choice

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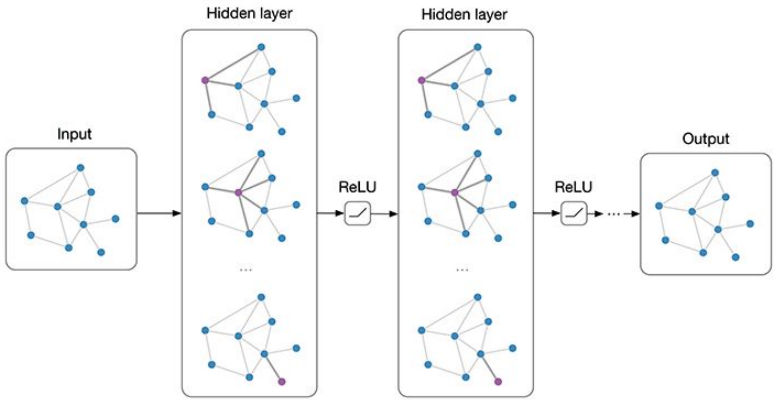
- Specifically, switching between S&G kernel and SpMM kernel based on input graph's at runtime.



Multi-layer Graph Convolutional Network (GCN) with first-order filters.

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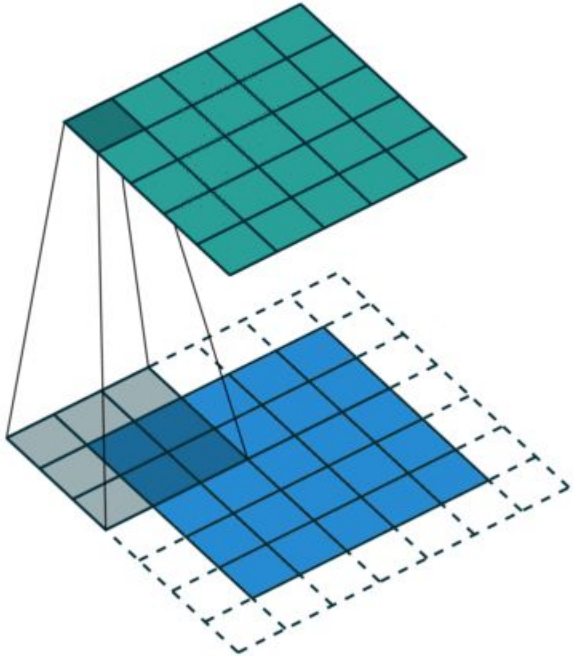
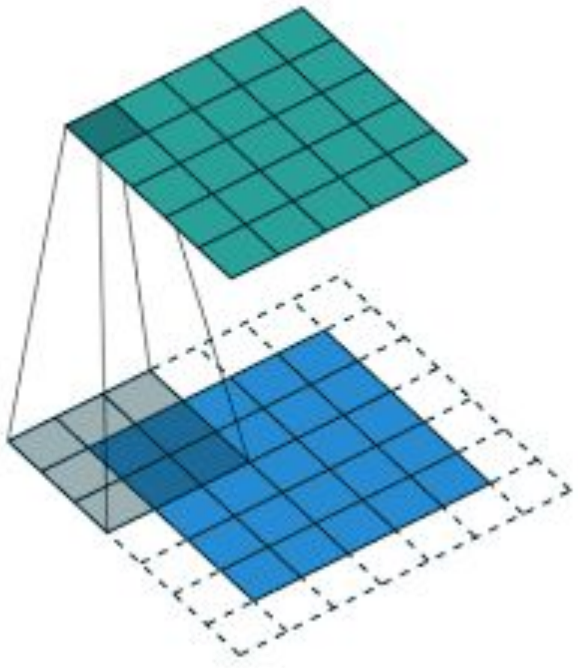
2D Convolution Versus Graph Convolution





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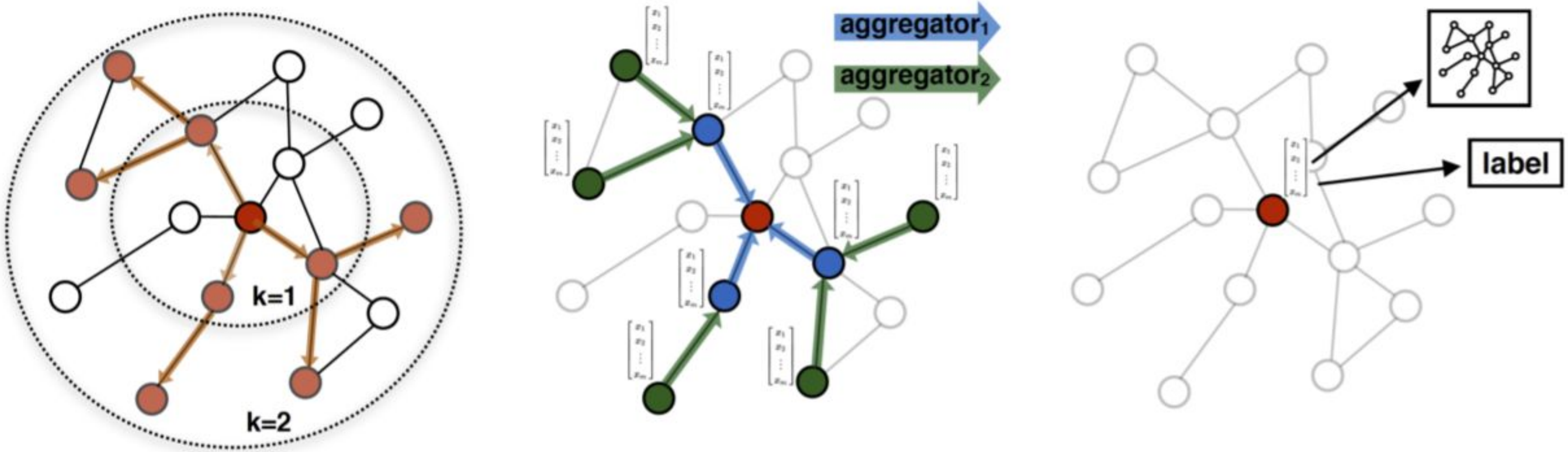

1. Sample neighborhood

2. Aggregate feature information from neighbors

3. Predict graph context and label using aggregated information

Mathematical Formulation of GCN

- SpMM (1)(2)
- SAG (3)

- Every neural network layer can then be written as a non-linear function

$$H^{(l+1)} = f(H^{(l)}, A)\,,$$

with $H^{(0)} = X$ and $H^{(L)} = Z$ (or z for graph-level outputs), L being the number of layers. The specific models then differ only in how $f(\cdot, \cdot)$ is chosen and parameterized.

- As an example, let's consider the following very simple form of a layer-wise propagation rule:

$$f(H^{(l)}, A) = \sigma\left(AH^{(l)}W^{(l)}\right)\,,$$

where $W^{(l)}$ is a weight matrix for the l-th neural network layer and $\sigma(\cdot)$ is a non-linear activation function like the ReLU. Despite its simplicity this model is already quite powerful (we'll come to that in a moment).

- $$a_v^{k+1} = Aggregate^{k+1}(h_u^{k+1} | u \in Neighbor(v))$$
$$h_v^{k+1} = Update^{k+1}(a_v^{k+1}, h_v^k)$$

https://tkipf.github.io/graph-convolutional-networks/

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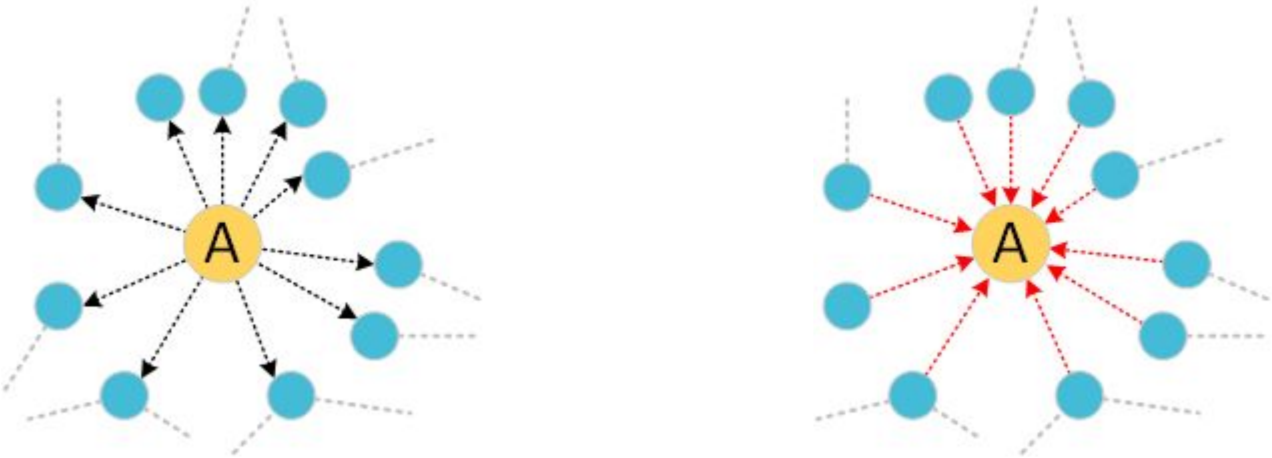
Scatter & Gather (SAG)

- Originated from graph processing, such as, PageRank, BFS.
- Push (conflicting-write) Vs. Pull (irregular-read)



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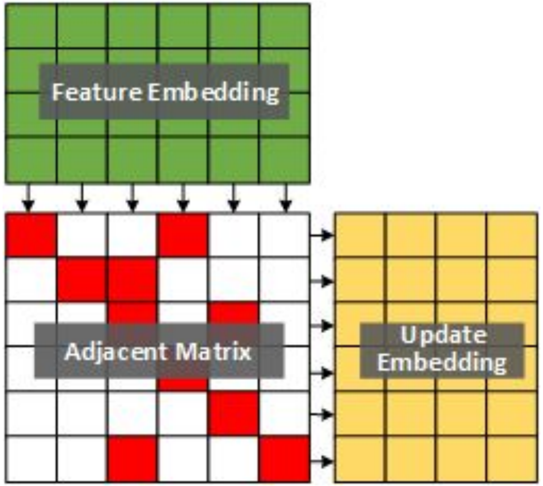
Sparse Matrix-Matrix Multiplication (SpMM)

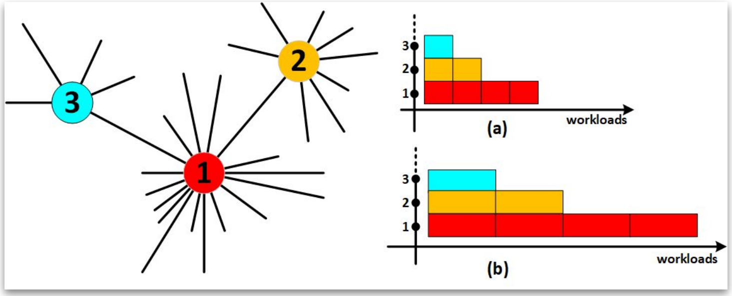
- Adapted from GraphBLAS-SpMV[1]
- Used for SUM-based Aggregation.

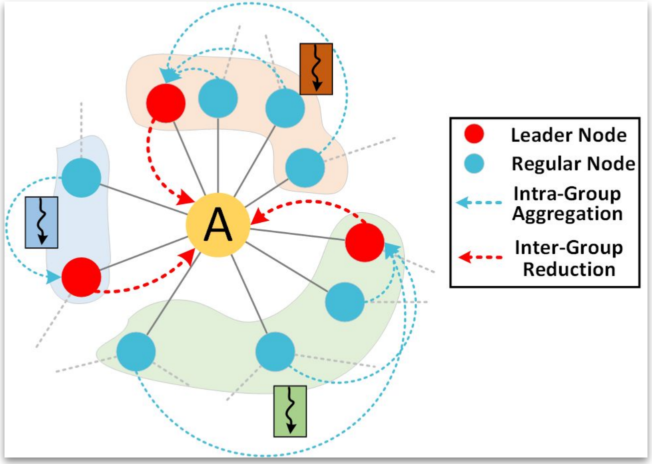


[1] http://graphblas.org/index.php?title=Graph_BLAS_Forum

Kernel Optimization

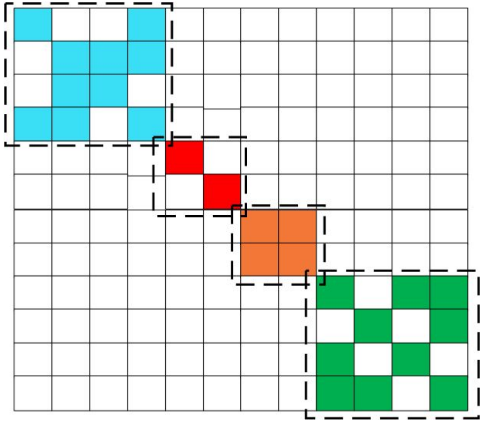
Group-based Neighbor Partitioning

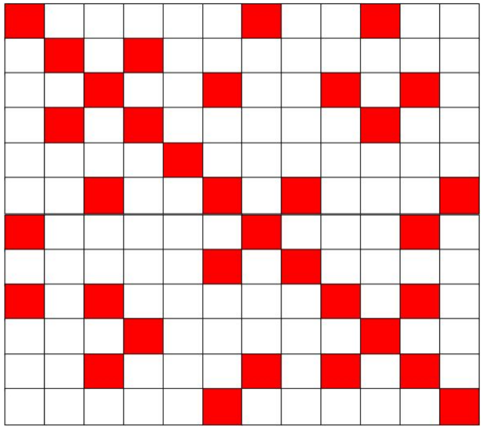




Kernel Choice

- Block-diagonal graph-- SpMM (top right).
- Random irregular graph -- SAG (bottom right).





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Implementation Details, list of wrapper choices

- Numba
- PyCuda
- scikit-CUDA
- SWIG
- Pytorch
- etc…..

Implementation Details, list of wrapper choices

- Numba (runtime compiler specifically optimize for math numpy code)
- PyCuda (Full CUDA API in Python, GC, Try-Catch CUDA errors, etc)
- scikit-CUDA (similar to PyCuda, only PyCuda is backed by Nvidia)
- SWIG (Simple Wrapper Interface Generator, statically compiled .o shared library)
- Pytorch (Augo-grad)
- etc…..

Python Wrapper Variant -- PyTorch

- Allow easy integrations of mixed CUDA, C++, Python code.

```python
from setuptools import setup, Extension
from torch.utils import cpp_extension

setup(name='lltm_cpp',
      ext_modules=[cpp_extension.CppExtension('lltm_cpp', ['lltm.cpp'])],
      cmdclass={'build_ext': cpp_extension.BuildExtension})
```

```cpp
PYBIND11_MODULE(TORCH_EXTENSION_NAME, m) {
  m.def("forward", &lltm_forward, "LLTM forward");
  m.def("backward", &lltm_backward, "LLTM backward");
}
```

```python
class LLTMFunction(torch.autograd.Function):
    @staticmethod
    def forward(ctx, input, weights, bias, old_h, old_cell):
        outputs = lltm_cpp.forward(input, weights, bias, old_h, old_cell)
        new_h, new_cell = outputs[:2]
        variables = outputs[1:] + [weights]
        ctx.save_for_backward(*variables)

        return new_h, new_cell
```

Python layer

```cpp
std::vector<torch::Tensor> lltm_cuda_forward(
    torch::Tensor input,
    torch::Tensor weights,
    torch::Tensor bias,
    torch::Tensor old_h,
    torch::Tensor old_cell) {
  auto X = torch::cat({old_h, input}, /*dim=*/1);
  auto gates = torch::addmm(bias, X, weights.transpose(0, 1));

  const auto batch_size = old_cell.size(0);
  const auto state_size = old_cell.size(1);

  auto new_h = torch::zeros_like(old_cell);
  auto new_cell = torch::zeros_like(old_cell);
  auto input_gate = torch::zeros_like(old_cell);
  auto output_gate = torch::zeros_like(old_cell);
  auto candidate_cell = torch::zeros_like(old_cell);

  const int threads = 1024;
  const dim3 blocks((state_size + threads - 1) / threads, batch_size);

  AT_DISPATCH_FLOATING_TYPES(gates.type(), "lltm_forward_cuda", ([&] {
    lltm_cuda_forward_kernel<scalar_t><<<blocks, threads>>>(
        gates.data<scalar_t>(),
        old_cell.data<scalar_t>(),
        new_h.data<scalar_t>(),
        new_cell.data<scalar_t>(),
        input_gate.data<scalar_t>(),
        output_gate.data<scalar_t>(),
        candidate_cell.data<scalar_t>(),
        state_size);
  }));

  return {new_h, new_cell, input_gate, output_gate, candidate_cell, X, gates};
}
```

C++ layer

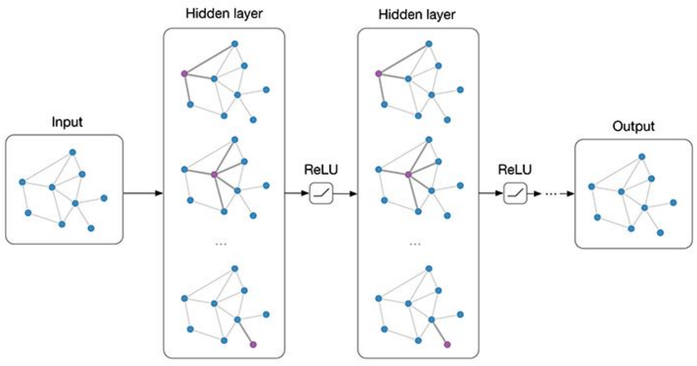
```cpp
template <typename scalar_t>
__global__ void lltm_cuda_forward_kernel(
    const scalar_t* __restrict__ gates,
    const scalar_t* __restrict__ old_cell,
    scalar_t* __restrict__ new_h,
    scalar_t* __restrict__ new_cell,
    scalar_t* __restrict__ input_gate,
    scalar_t* __restrict__ output_gate,
    scalar_t* __restrict__ candidate_cell,
    size_t state_size) {
  const int column = blockIdx.x * blockDim.x + threadIdx.x;
  const int index = blockIdx.y * state_size + column;
  const int gates_row = blockIdx.y * (state_size * 3);
  if (column < state_size) {
    input_gate[index] = sigmoid(gates[gates_row + column]);
    output_gate[index] = sigmoid(gates[gates_row + state_size + column]);
    candidate_cell[index] = elu(gates[gates_row + 2 * state_size + column]);
    new_cell[index] =
        old_cell[index] + candidate_cell[index] * input_gate[index];
    new_h[index] = tanh(new_cell[index]) * output_gate[index];
  }
}
```

CUDA Layer

https://pytorch.org/tutorials/advanced/cpp_extension.html

Our Project Recap and Our Choice of Wrapper

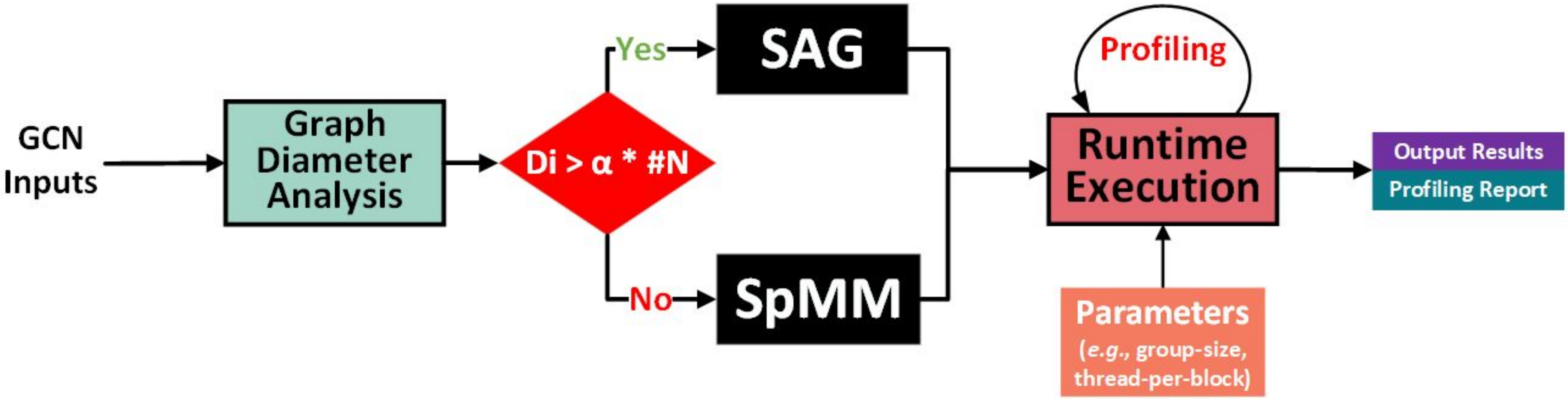
- Implement a runtime GCN library that looks at input graph's characteristic to make decisions on what specific kernels to call.
- Specifically, switching between S&G kernel and SpMM kernel based on input graph's at runtime.
- PyTorch wrapper.



Multi-layer Graph Convolutional Network (GCN) with first-order filters.

PyTorch

Overall Architecture



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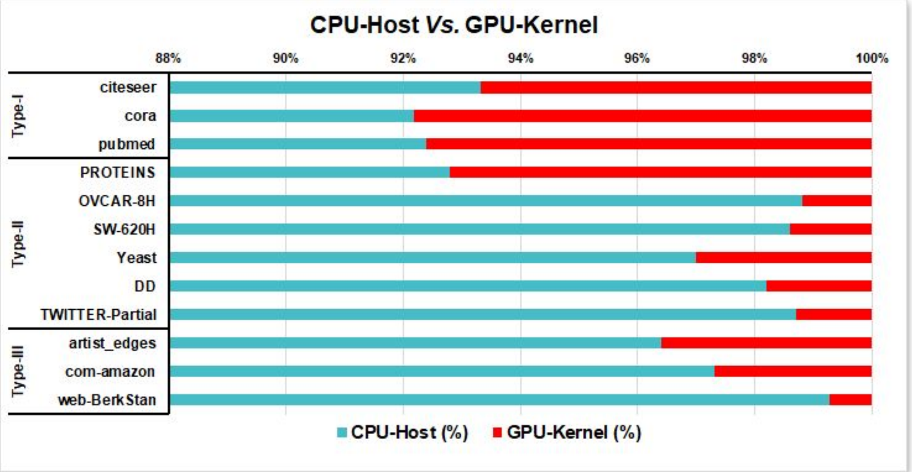
- Implemented a runtime system for Graph Convolutional Networks (GCN).
- **Profiled performance difference and runtime bottleneck.**

Tools & Datasets

- **[Host]** Xeon 4110 Silver 8 core, 64GB DDR4 RAM.
- **[GPU]** Nvidia Quadro P6000 (24GB GDDR5X).
- **`perf_counter()`** for CPU runtime profiling.
- **`NVProf`** for GPU kernel runtime profiling.

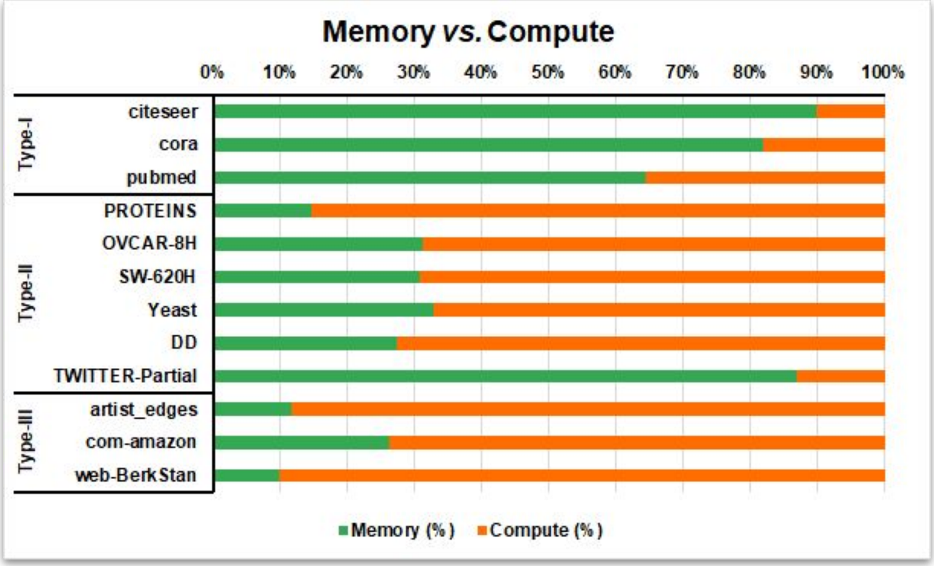
	Dataset	Node	Edges	Dim	Classes	Avg Degree
Type I	Citeseer	3,327	9,464	3703	6	2.84
	Cora	2,708	10,858	1433	7	4.01
	Pubmed	19,717	88,676	500	3	4.50
	PPI	56,944	818,716	50	121	14.38
Type II	PROTEINS_full	43,471	162,088	29	2	3.73
	OVCAR-8H	1,890,931	3,946,402	66	2	2.09
	Yeast	1,714,644	3,636,546	74	2	2.12
	DD	334,925	1,686,092	89	2	5.03
	TWITTER-Partial	580,768	1,435,116	1323	2	2.47
	SW-620H	1,889,971	3,944,206	66	2	2.09
Type III	amazon0505	410,236	4,878,875	96	22	11.89
	artist	50,515	1,638,396	100	12	32.43
	com-amazon	334,863	1,851,744	96	22	5.53
	soc-BlogCatalog	88,784	2,093,195	128	39	23.58
	amazon0601	403,394	3,387,388	96	22	8.40

Runtime Decomposition

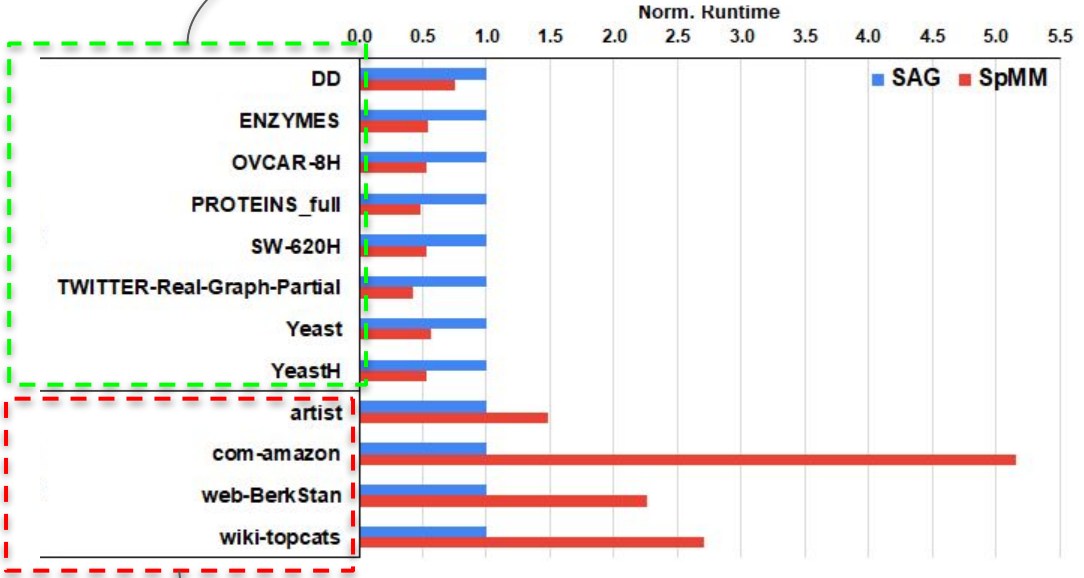


- Intelligent Kernel Switch
  + Graph Preprocessing Cost
- GPU Kernel Cost

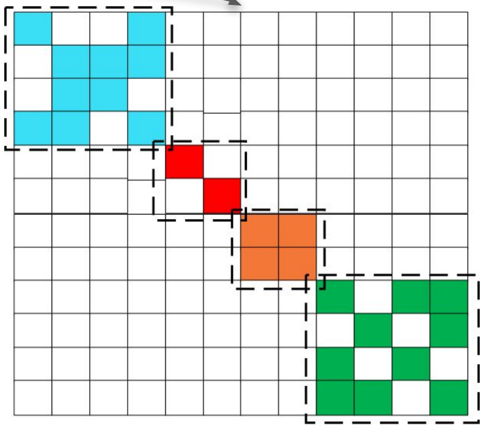
- **Memory**
  - **Allocation**
  - **CPU Host <-> GPU**

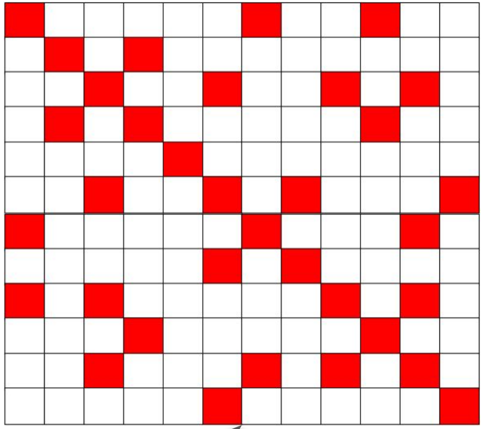


SpMM vs SAG

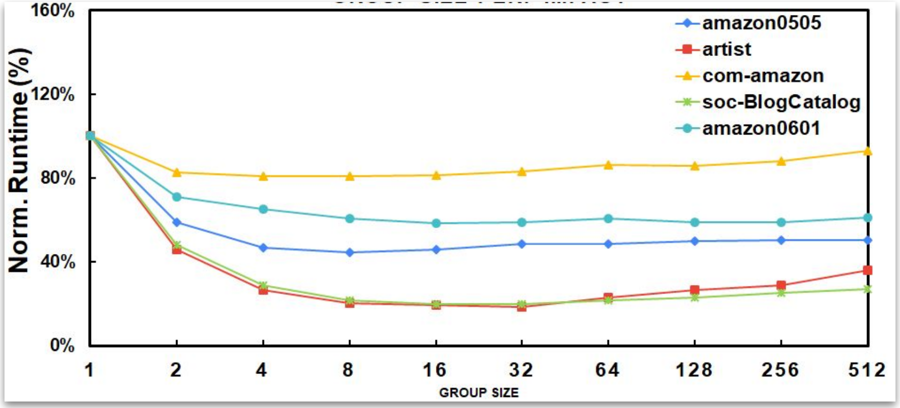


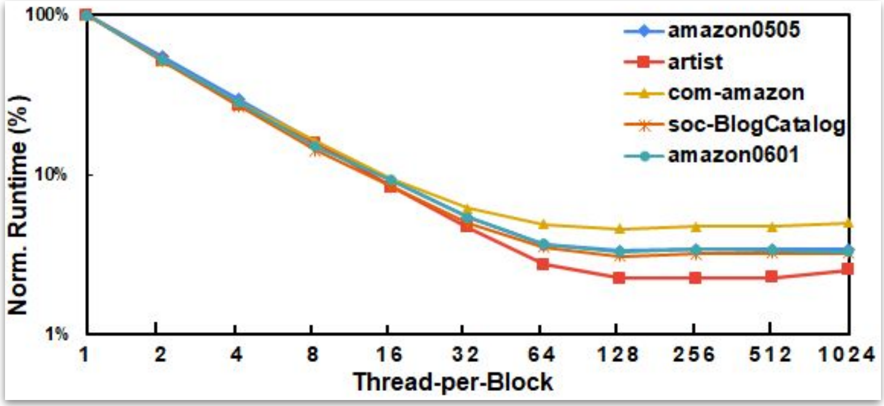
Note: we normalize runtime of SpMM *w.r.t.* SAG

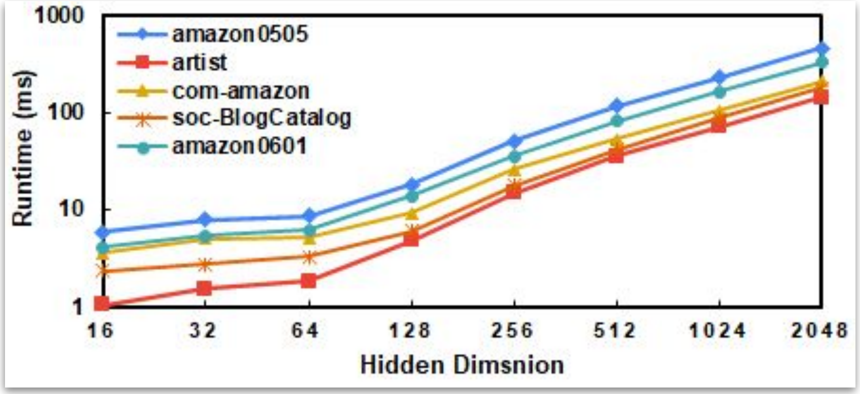




Case Studies







Conclusion

- Surveyed different runtime systems / python wrappers popularized from the recent “AI” wave.

- Built a GCN runtime on GPUs.
  - Scatter and Gather (SAG) Kernel
  - Sparse matrix multiplication (SpMM) kernel
  - Pytorch mixed CUDA/C++/Python wrapper
  - Runtime decision making on graph characteristics. **AUTO** and **Manual** Kernel Selection.
  - Performance tuning options. **Group-size** and **thread-per-block**.

- A complete profiling toolset (Profiler + Report Generator) for CPU host and GPU kernel evaluation.

Thank You

Q&A

Data Science Workhorse -- NumPy

- All-in-one solution for data storage, matrix/tensor math.

```
>>> A = np.array( [[1,1],
...             [0,1]] )
>>> B = np.array( [[2,0],
...             [3,4]] )
>>> A * B                       # elementwise product
array([[2, 0],
       [0, 4]])
>>> A @ B                       # matrix product
array([[5, 4],
       [3, 4]])
>>> A.dot(B)                    # another matrix product
array([[5, 4],
       [3, 4]])
```

```
>>> b = np.arange(12).reshape(3,4)
>>> b
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>>
>>> b.sum(axis=0)                            # sum of each column
array([12, 15, 18, 21])
>>>
>>> b.min(axis=1)                            # min of each row
array([0, 4, 8])
>>>
>>> b.cumsum(axis=1)                         # cumulative sum along each row
array([[ 0,  1,  3,  6],
       [ 4,  9, 15, 22],
       [ 8, 17, 27, 38]])
```

How Runtime System Helped in this Revolution?

- Adding specific runtime compiling supports for these people. Study their programming habits / code usage pattern, and design specific runtime optimization strategies accordingly. Numba is a good example.

Python Wrapper Variant -- Numba

- A Just in Time compiler that works best on python code that uses NumPy arrays, functions, and loops.
- Use python decorators as hint to Numba compiler.
- Unlike Pytorch, TensorFlow, etc, no support for autograd.

```
from numba import jit
import numpy as np

x = np.arange(100).reshape(10, 10)

@jit(nopython=True) # Set "nopython" mode for best performance, equivalent to @njit
def go_fast(a): # Function is compiled to machine code when called the first time
    trace = 0.0
    for i in range(a.shape[0]):   # Numba likes loops
        trace += np.tanh(a[i, i]) # Numba likes NumPy functions
    return a + trace              # Numba likes NumPy broadcasting

print(go_fast(x))
```

https://numba.pydata.org/numba-doc/latest/user/5minguide.html

Matrix Multiplication Optimization As An Example

- Naive iterative matrix multiplication algorithm involves two big for loops. Compute for one C_ij at one time step.

$$c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}.$$

- Input: matrices A and B
- Let C be a new matrix of the appropriate size
- For i from 1 to n:
    - For j from 1 to p:
        - Let $\mathrm{sum} = 0$
        - For k from 1 to m:
            - Set $\mathrm{sum} \leftarrow \mathrm{sum} + A_{ik} \times B_{kj}$
        - Set $C_{ij} \leftarrow \mathrm{sum}$
- Return C

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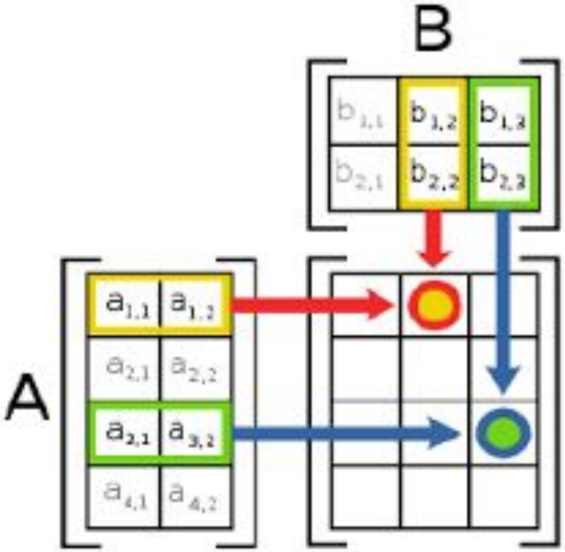
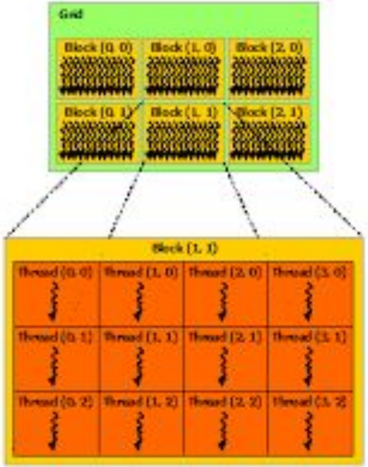


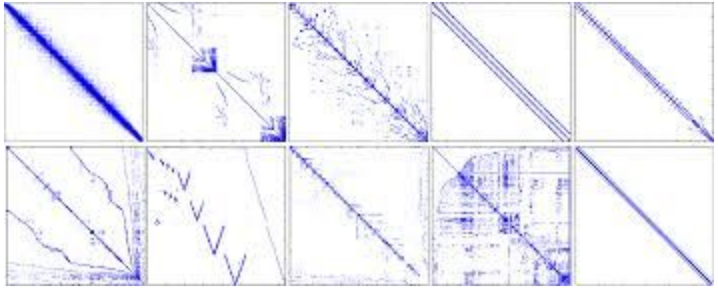
- Can be accelerated using CUDA. Compute all C_ij at the same time. Put A and B in shared GPU memory. Each thread writes into one C_ij.

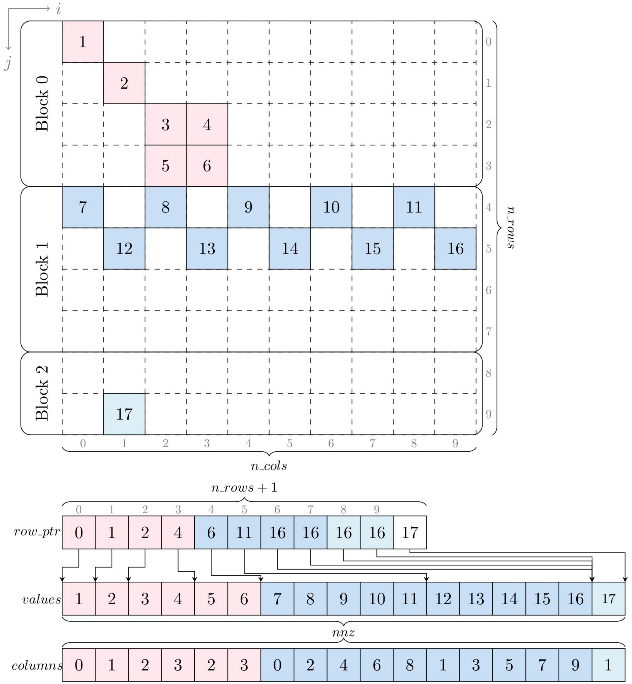


Matrix Multiplication Optimization As An Example

- Can also introduce parallelism by using block matrix multiplication and exploiting sparsity of a matrix, etc.

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{pmatrix}$$





Mathematical Formulation of GCN

- Every neural network layer can then be written as a non-linear function

$$H^{(l+1)} = f(H^{(l)}, A)\,,$$

with $H^{(0)} = X$ and $H^{(L)} = Z$ (or z for graph-level outputs), L being the number of layers. The specific models then differ only in how $f(\cdot, \cdot)$ is chosen and parameterized.

- As an example, let's consider the following very simple form of a layer-wise propagation rule:

$$f(H^{(l)}, A) = \sigma\left(AH^{(l)}W^{(l)}\right)\,,$$

where $W^{(l)}$ is a weight matrix for the l-th neural network layer and $\sigma(\cdot)$ is a non-linear activation function like the ReLU. Despite its simplicity this model is already quite powerful (we'll come to that in a moment).

Think of A as an Adjacency Matrix describing your Graph. W is the trainable weight.

https://tkipf.github.io/graph-convolutional-networks/

Python Wrapper Variant -- PyCuda

- Full NVIDIA CUDA API in Python.
- Work with Numpy
- Garbage collector support. Object cleanup tied to object’s lifetime.
- Automatic Error Checking. Python exceptions. More Traceable Errors.

```
import pycuda.autoinit
import pycuda.driver as drv
import numpy

from pycuda.compiler import SourceModule
mod = SourceModule("""
__global__ void multiply_them(float *dest, float *a, float *b)
{
  const int i = threadIdx.x;
  dest[i] = a[i] * b[i];
}
""")

multiply_them = mod.get_function("multiply_them")

a = numpy.random.randn(400).astype(numpy.float32)
b = numpy.random.randn(400).astype(numpy.float32)

dest = numpy.zeros_like(a)
multiply_them(
        drv.Out(dest), drv.In(a), drv.In(b),
        block=(400,1,1), grid=(1,1))

print dest-a*b
```

https://documen.tician.de/pycuda/

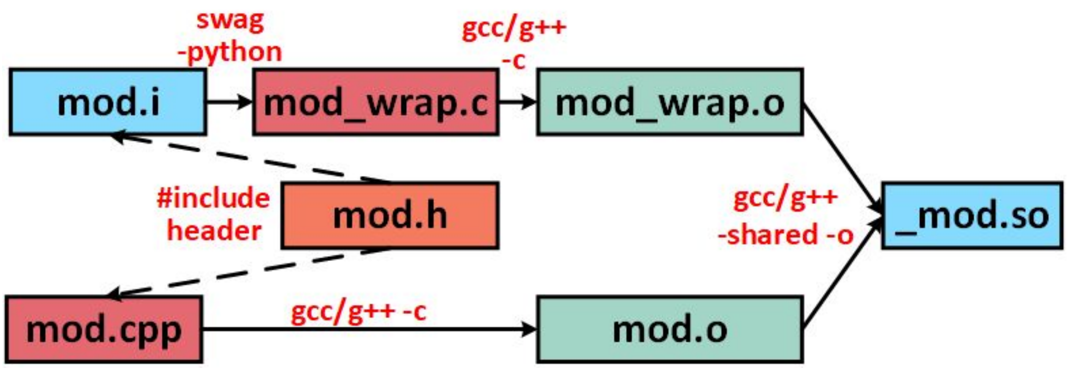
Python Wrapper Variant -- scikit-CUDA

- Similar to PyCUDA (backed by Nvidia).
- Less developed.
- With scikit-learn, SciPy open source community.

https://scikit-cuda.readthedocs.io/en/latest/

Python Wrapper Variant -- SWIG

- Generic Wrapper. Statically Compiled as a .so library that you can use at runtime.



https://intermediate-and-advanced-software-carpentry.readthedocs.io/en/latest/c++-wrapping.html

Python Wrapper Variant -- PyTorch

- One of the most popular Auto-grad Frameworks among Machine Learning researchers.
- Torch tensor objects wrap around Numpy objects with Auto-grad support.

```
>>> torch.tensor([[1., -1.], [1., -1.]])
tensor([[ 1.0000, -1.0000],
        [ 1.0000, -1.0000]])
>>> torch.tensor(np.array([[1, 2, 3], [4, 5, 6]]))
tensor([[ 1,  2,  3],
        [ 4,  5,  6]])
```

```
>>> cuda0 = torch.device('cuda:0')
>>> torch.ones([2, 4], dtype=torch.float64, device=cuda0)
```

```
>>> x = torch.tensor([[1., -1.], [1., 1.]], requires_grad=True)
>>> out = x.pow(2).sum()
>>> out.backward()
>>> x.grad
tensor([[ 2.0000, -2.0000],
        [ 2.0000,  2.0000]])
```

d(x^2)/dx = 2x

https://pytorch.org/docs/stable/tensors.html

Implementation Details, list of wrapper choices

- Numba (runtime compiler specifically optimize for Numpy math code, GPU)
- PyCuda
- scikit-CUDA
- SWIG
- Pytorch
- etc…..

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- PyCuda (Full CUDA API in Python, GC, Try-Catch CUDA errors, etc)
- scikit-CUDA (similar to PyCuda, only PyCuda is backed by Nvidia)
- SWIG (Simple Wrapper Interface Generator, statically compiled .o shared library)
- Pytorch
- etc…..