Deep Learning and Quantum Many Body Systems

A programming guide

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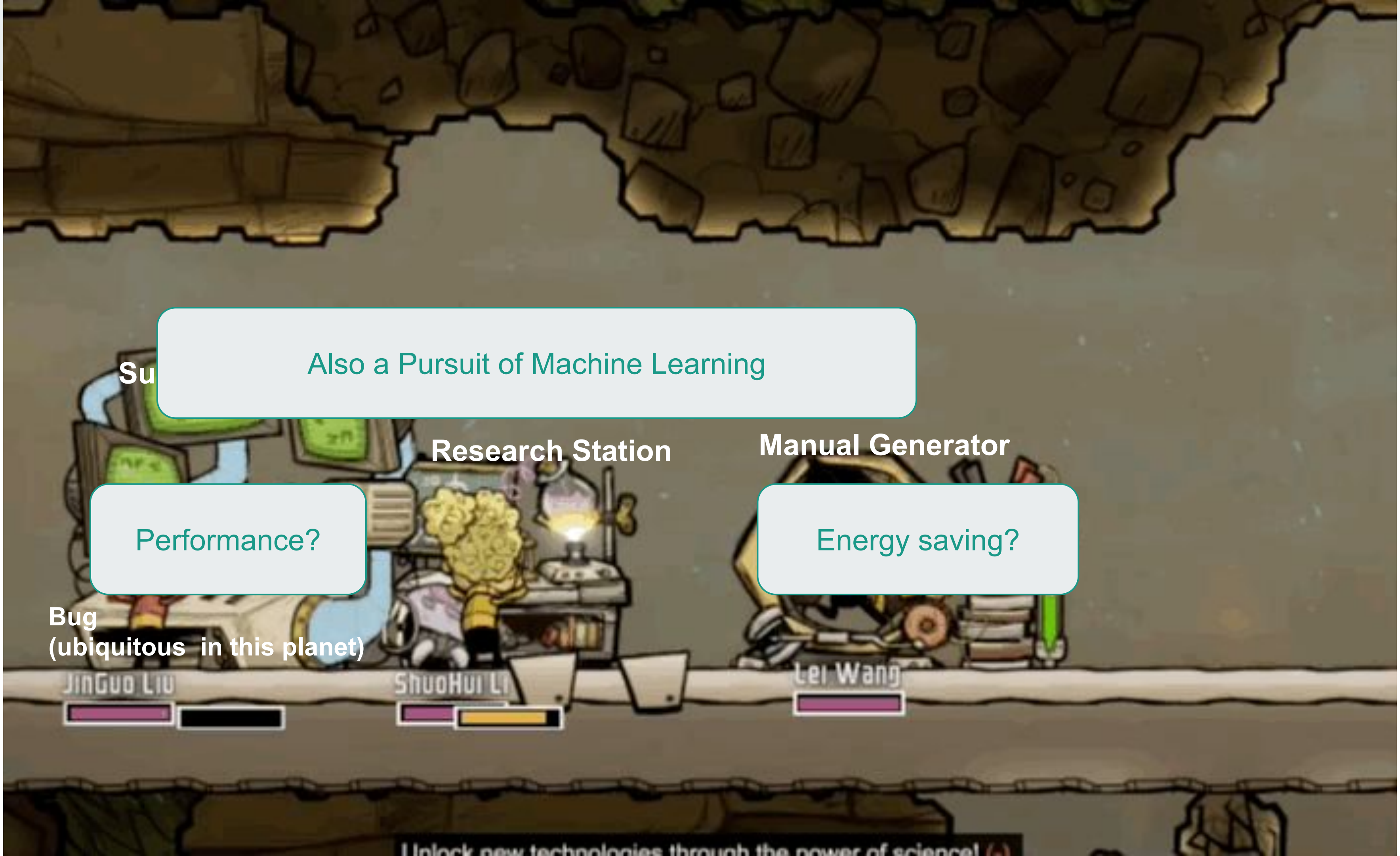
Setup your workplace

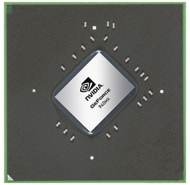
Following the guide
https://github.com/GiggleLiu/marburg/

If you cloned this repository or lecture notes days before, pull for updates please!



Also a Pursuit of Machine Learning
Su
Research Station
Manual Generator
Performance?
Energy saving?
Bug
(ubiquitous in this planet)
JinGuo Liu
ShuoHui Li
Lei Wang

Use the Right Device



How to calculate FLOPS?
See notebook *gpu/hardware.ipynb* in our github repository for an example.

	CPU	Graphics Card
	Intel Core i5-7200U (15 W) (Ultra-low power)	NVIDIA GeForce 940MX (23 W)
Parallelism	2 cores (2.5GHZ), AVX2 SIMD	384 CUDA cores (1.189GHZ)
	40 GFLOPS	913 GFLOPS

AVX2 acceleration of saxpy function

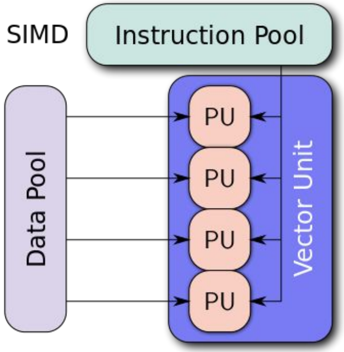
$$\mathbf{y} = a\mathbf{x} + \mathbf{y}$$

Not vectorized

```
void saxpy(int n, float a, float *x, float *y) {
    for (int i=0; i<n; i++)
        y[i] = a*x[i] + y[i];
}
```

AVX2 vectorized

```
void saxpy(int n, float a, float *x, float *y){
    __m256 x_vec, y_vec, a_vec, res_vec;      //define the registers used
    a_vec = _mm256_set1_ps(a); // Vector of 8 alpha values
    for (int i=0; i<n; i+=8) {
        x_vec = _mm256_loadu_ps(&x[i]); // Load 8 values from X
        y_vec = _mm256_loadu_ps(&y[i]); // Load 8 values from Y
        res_vec = _mm256_fmadd_ps(a_vec, x_vec, y_vec); // Compute
        _mm256_store_ps(&y[i], res_vec);
    }
}
```



Load data to SIMD register

Read result from SIMD register

https://devblogs.nvidia.com/easy-introduction-cuda-c-and-c/

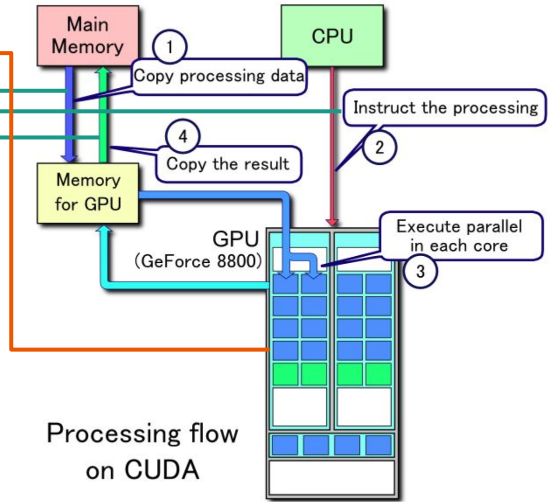
CUDA programming model

device code

```
__global__ void saxpyDevice(int n, float a, float *x, float *y){
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    if (i < n) y[i] = a*x[i] + y[i];
}
```

host code

```
void saxpy(int n, float a, float *x, float *y){
    float *d_x, *d_y;

    cudaMalloc(&d_x, n*sizeof(float));
    cudaMalloc(&d_y, n*sizeof(float));

    cudaMemcpy(d_x, x, n*sizeof(float), cudaMemcpyHostToDevice);
    cudaMemcpy(d_y, y, n*sizeof(float), cudaMemcpyHostToDevice);

    // Perform SAXPY on GPU
    saxpyDevice<<<(n+255)/256, 256>>>(n, 2.0f, d_x, d_y);

    cudaMemcpy(y, d_y, n*sizeof(float), cudaMemcpyDeviceToHost);

    cudaFree(d_x);
    cudaFree(d_y);
}
```



Free ourselves from low-level programming

Define the Computation $\xrightarrow{\text{lib}}$ Choose the device to run

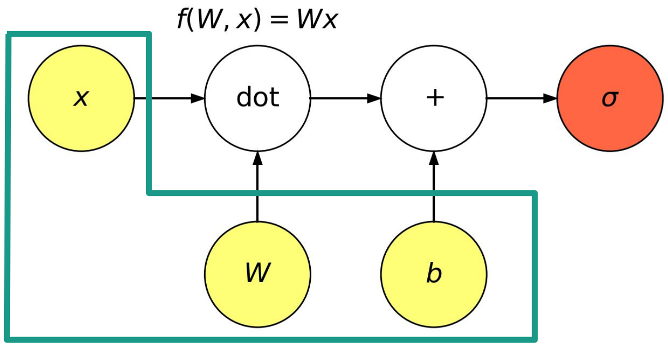
Computation graph

Neural network version of Feynman Diagram

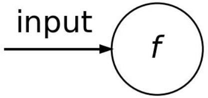
CPU/GPU(s)/TPU

An Example of Computation Graph

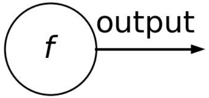
$$f(x) = \sigma(Wx + b)$$



load data to graph



function argument



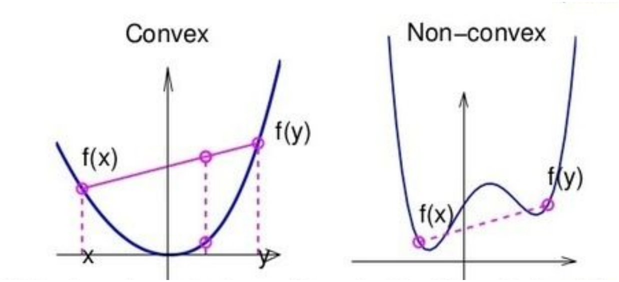
function output

A node knows how to compute its **derivative** w.r.t each argument (edge).

Can be used to $\boxed{\text{train a NN}}$ Loss function

Choromanska, Anna, et al. "The loss surfaces of multilayer networks." Artificial Intelligence and Statistics. 2015.

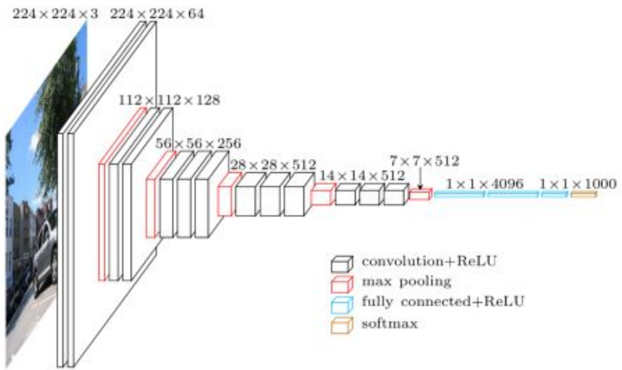
Losses Expressed as Computation Graphs



theory reality

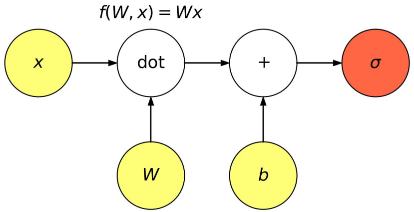
Convex optimization model

VGG-16 network (138 M parameters)



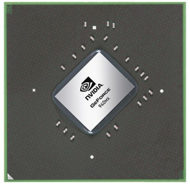
Not to find the global minima, but to obtain a low enough loss efficiently.

So Far



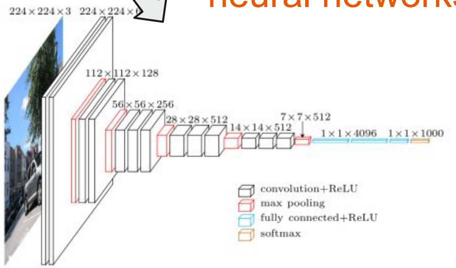
Computation Graphs

Provide unified framework to use computation resources



Devices

Provide efficient training of neural networks



Neural Networks

2:50

Hands on time

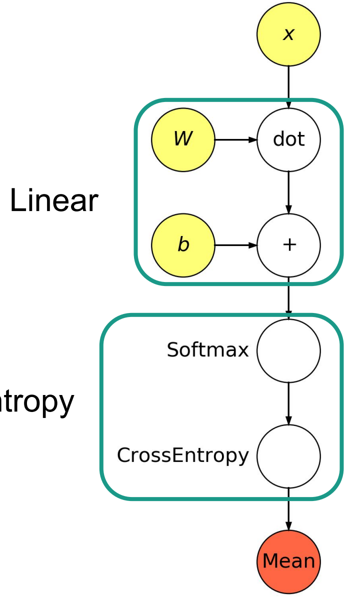
with numpy:

build functions used in computation graphs

conquer digits classification problem

★ build your own computation graph node

A Digit Classification Problem

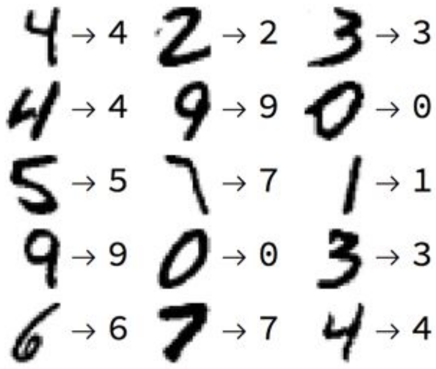


Generate One hot labels

Comparison

Target: Correctly assign labels, e.g.

Softmax: [0.1, 0, 0, 0, 0.8, 0.1, 0, 0, 0, 0]
Label: [0 , 0, 0, 0, 1 , 0 , 0, 0, 0, 0]



A typical Application

Detect Phase Transition

https://goo.gl/DZtidF

Solution

$$y = \sum_i (\log(\sum_j e^{x_j}) - x_i) p_i$$

$$\frac{\partial \mathcal{L}}{\partial x_i} = \frac{\partial \mathcal{L}}{\partial y} \left(\frac{e^{x_i}}{\sum_j e^{x_j}} - p_i \right)$$

State of Art Python Neural Network Libraries

TensorFlow™

Developer	Google Brain Team
Initial release	November 9, 2015
Stable release	1.5.0 / January 26, 2018
Repository	github.com/tensorflow/tensorflow
Written in	Python, C++, CUDA
Platform	Linux, macOS, Windows, Android
License	Apache 2.0 open source license
Website	www.tensorflow.org

PYTORCH

Developer	Facebook's AI research group
Initial release	October 2016
Stable release	0.3.0 / 5 December 2017
Repository	github.com/pytorch/pytorch
Written in	Python, C, CUDA
Platform	Linux, macOS
Website	pytorch.org

Major difference

TensorFlow	PyTorch
static graph	dynamic graph

Static and Dynamic Graphs

Static graphs

Define the graph, feed data into the graph, run on its VM and get output.

- Platform independent
- Optimize the graph before running

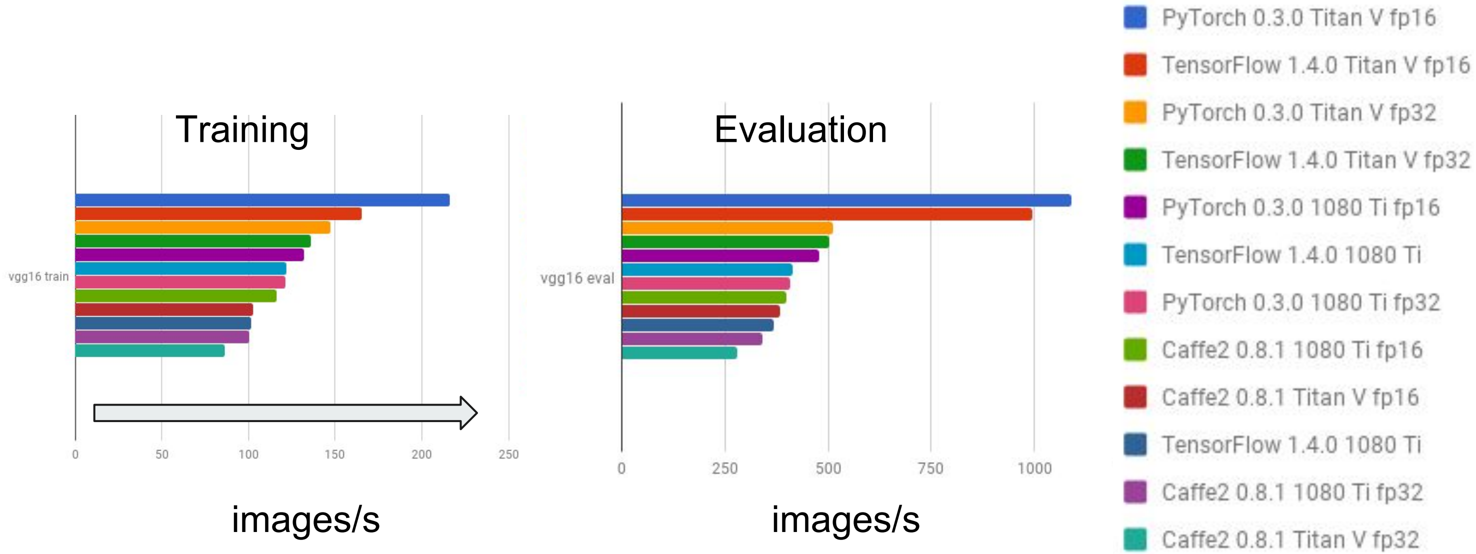
Dynamic graphs

Build graph while running, remember the graph for back propagation.

- Pythonic control flow
- Rebuild the graph in each run, more flexible

https://github.com/u39kun/deep-learning-benchmark

A Benchmark on Performance



VGG 16 network

Pytorch used in this tutorial

Advantages:

Performance
easy for extensions
easy to debug
friendly to beginners

Disadvantages:

No complex number support
Sometimes being unstable and buggy

PYTORCH

http://pytorch.org/

Notebook

https://goo.gl/8Caymh

local: nice.py

Hands on time

Notebook with Solution
https://goo.gl/FhAHRZ

with pytorch:

build a NICE network

solve a sampling problem

★ build a RealNVP network to do it better

A typical application
Accelerate Monte Carlo sampling for ϕ_4 Model

Experience CUDA acceleration without having Nvidia GPUs

Open colab notebook

Edit

- Notebook settings
  - Hardware accelerator
  - Choose GPU

Hands on time

with pytorch and GPU:

build a restricted Boltzmann machine (RBM)

write a digits generative model

★ recover a broken image

RBM as a wave function ansatz for VMC

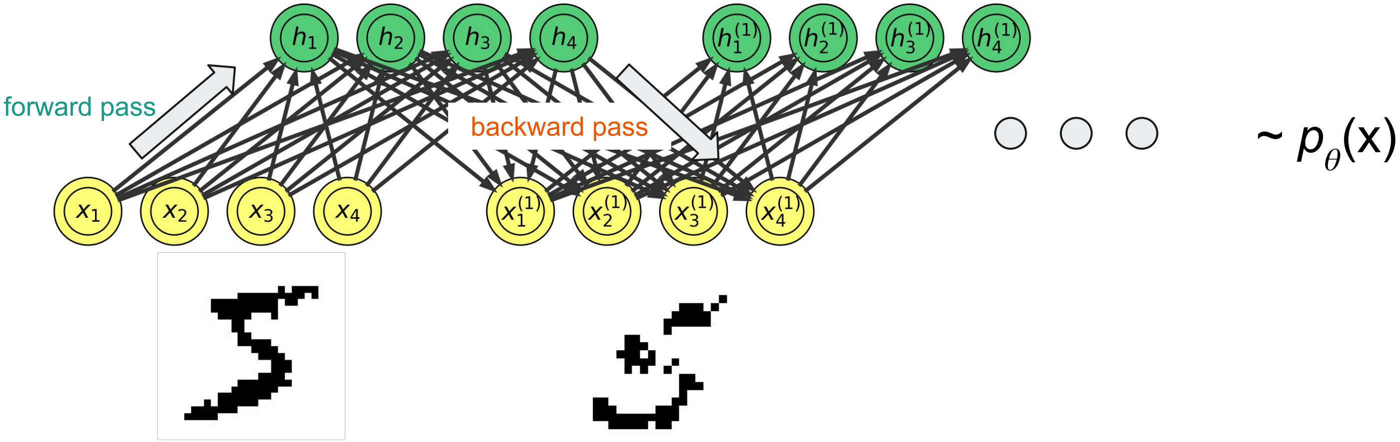
https://goo.gl/d7kPzy

local: rbm_generation.py

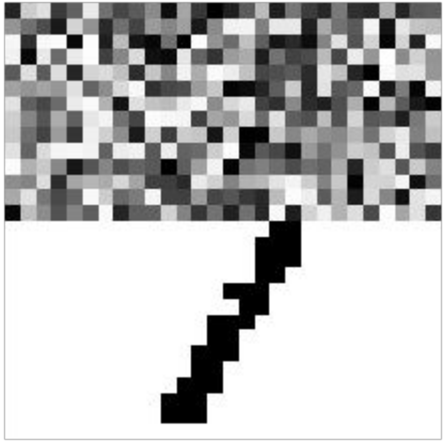
Miguel, A., & Hinton, G. E. (n.d.). On Contrastive Divergence Learning, 0.

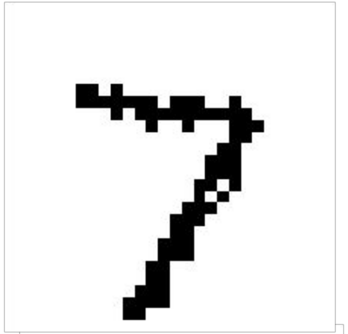
$$\frac{\partial \mathcal{L}}{\partial \theta} = \langle \frac{\partial E_\theta(x)}{\partial \theta} \rangle_{x \sim \mathcal{D}} - \langle \frac{\partial E_\theta(x)}{\partial \theta} \rangle_{x \sim p_\theta(x)}$$

Gibbs sampling process

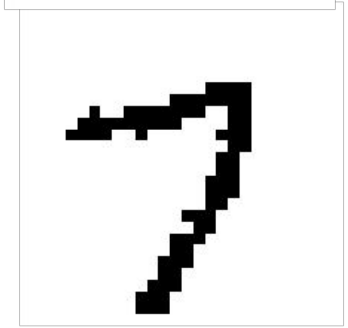


A Typical Result





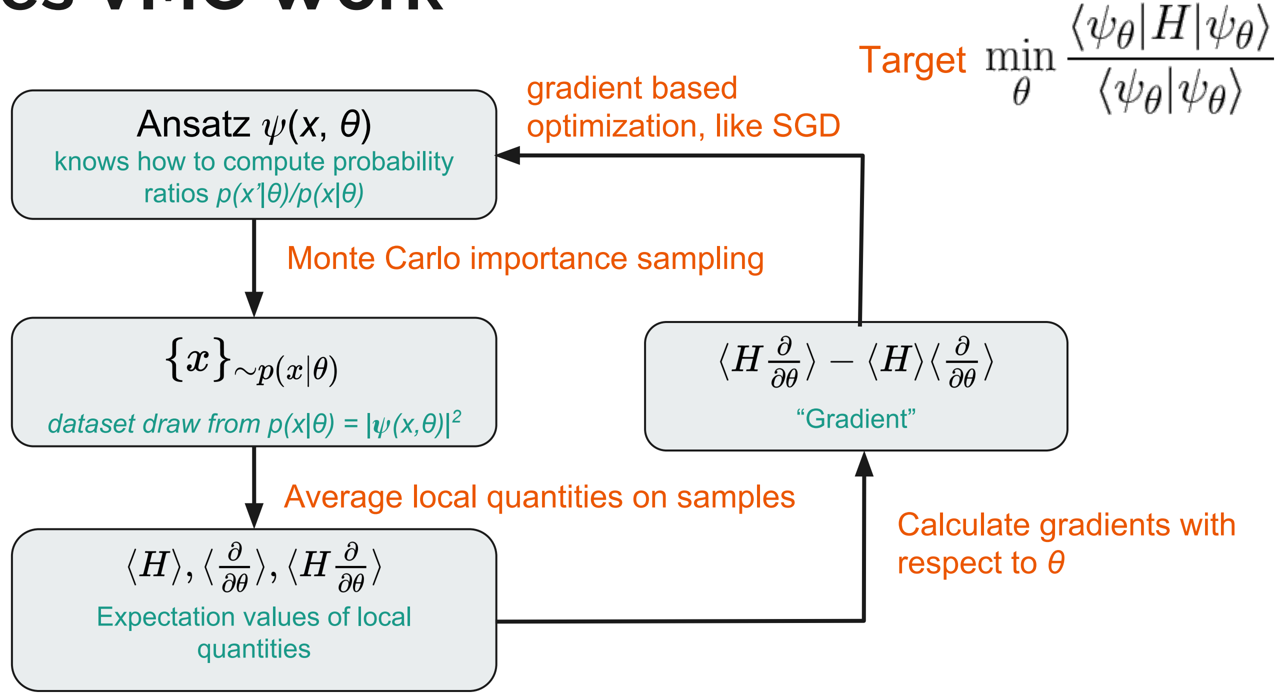
Original digit



Generated digit

Takahiro has already introduced it yesterday

How does VMC Work



$$\Delta_{\text{loc}}(x) = \frac{\partial \log \psi(x,\theta)}{\partial\theta}$$

$$E_{\text{loc}}(x) = \frac{\langle x | H | \psi(\theta) \rangle}{\langle x | \psi(\theta) \rangle}$$

$$\langle H \rangle = \langle E_{\text{loc}} \rangle_{\{x\}}$$

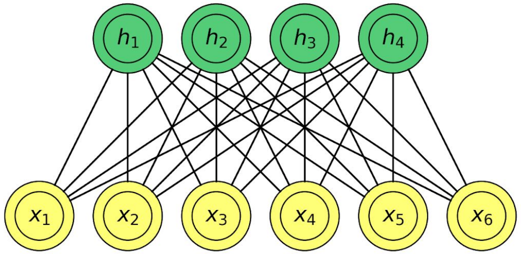
$$\langle \frac{\partial}{\partial\theta} \rangle = \langle \Delta_{\text{loc}} \rangle_{\{x\}}$$

Carleo, Giuseppe, and Matthias Troyer. "Solving the quantum many-body problem with artificial neural networks." Science 355.6325 (2017): 602-606.
Cai, Zi, and Jinguo Liu. "Approximating quantum many-body wave functions using artificial neural networks." Physical Review B 97.3 (2018): 035116.

https://goo.gl/vPFtdU

local: rbm_ansatz.py

RBM as a Wave Function Ansatz

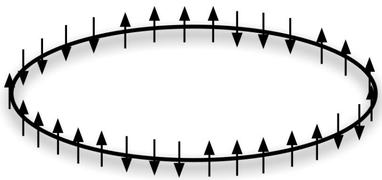


$$x_i = \pm 1$$

$$p(x|\theta) = e^{\sum_i a_i x_i} \prod_{i=1}^{M} 2\cosh(b_i + \sum_j W_{ij} x_j)$$

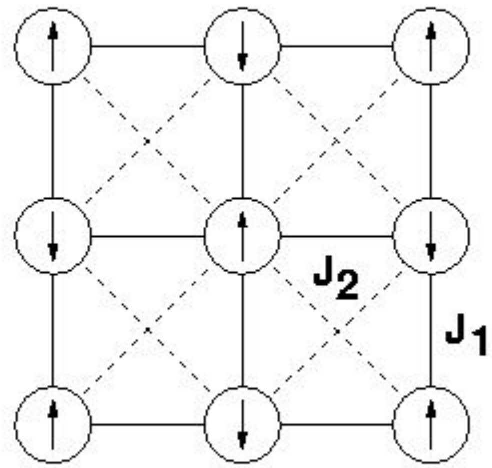
positive

$$p(x) \propto \langle x|\psi\rangle$$



$$H = J \sum_{i=1}^{N} S_i^z S_{i+1}^z - \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^+ S_{i+1}^-)$$

Ground State for Frustrated Quantum Spin Systems An Open Question yet



Thanks

Lei Wang

Being a level 12 scientist, Lei Wang's brain is filled with crazy ideas.

Shuo-Hui Li

Besides being strong at robotics and coding stuff, he has a bottomless stomach.

Jin-Guo Liu

Digging and coding are similar, they both produce bugs. Mole hands, coding speed + 50%.

More Slides

https://goo.gl/6d2sei

Setup your workplace

Local Setup

1. setup environment according to https://github.com/GiggleLiu/marburg/
2. clone notebooks to local host
   $ git clone
   https://github.com/GiggleLiu/marburg.git
3. run it
   $ cd winterchool/notebooks
   $ ipython notebook
4. Open computation_graph.ipynb

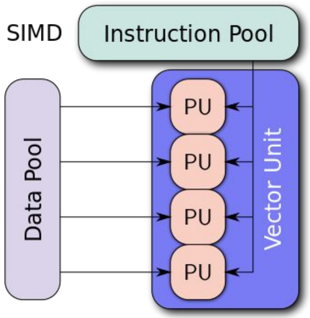
If you cloned this repository or lecture notes days before, pull for updates please!

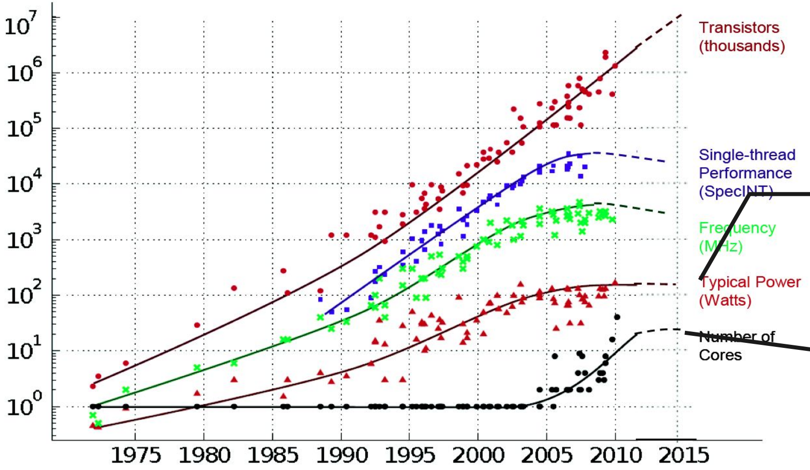
Online notebook

Google Collaborator + Google Drive
https://colab.research.google.com
https://drive.google.com

1. Sign in Google drive
2. Connect Google drive with Google Colaboratory
   a. right click on google drive page
   b. More
   c. Connect more apps
   d. search “Colaboratory” and “CONNECT
3. Open the online notebook link on top right
4. Click “open with colaboratory” on top
5. Save a copy of notebook to your google drive
6. Run/Edit this notebook

Two Trends in CPU manufacturing





Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten
Dotted line extrapolations by C. Moore

Lower Power Consumption

Intel Core i5-7200U

Ultra-low power

Parallelism to Increase Computation Speed

Multi-core CPUs

Single instruction, multiple data (SIMD)

Parallelism Extremists GPU

GPU Programming?
CUDA programming model (Nvidia)

	# Cores	Clock Speed	Memory
CPU (Intel Core i7-7700k)	4 (8 threads with hyperthreading)	4.4 GHz	Shared with system
CPU (Intel Core i7-6950X)	10 (20 threads with hyperthreading)	3.5 GHz	Shared with system
GPU (NVIDIA Titan Xp)	3840	1.6 GHz	12 GB GDDR5X
GPU (NVIDIA GTX 1070)	1920	1.68 GHz	8 GB GDDR5

Why convex optimization model works

Figure 6 compares SGD with SA.

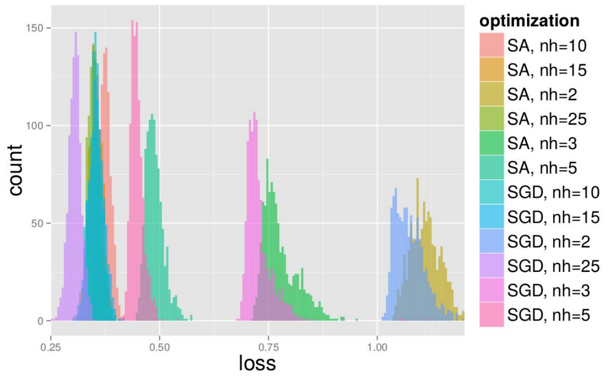


Figure 6: Test loss distributions for SGD and SA for different numbers of hidden units (nh).

- Deeper network: narrower loss distribution
- Global minima: overfit (fit too good for training set, can not be generalized to test set.)