# BLUE WATERS SUSTAINED PETASCALE COMPUTING



#### Presented By: Aaron D. Saxton, PhD









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# **Statistics Review**

- Simple  $y = m \cdot x + b$  regression
  - Least Squares to find m,b
  - With data set  $\{(x_i, y_i)\}_{i=1,\dots,n}$ 
    - Very special, often hard to measure  $y_i$
  - Let the error be
    - $R = \sum_{i=1}^{n} [(y_i (m \cdot x_i + b))]^2$
  - Minimize *R* with respect to *m* and *b*.
    - Simultaneously Solve
      - $R_m(m,b) = 0$
      - $R_b(m,b) = 0$
    - Linear System
- We will consider more general y = f(x)
  - $R_m(m,b) = 0$  and  $R_b(m,b) = 0$  may not be linear







# **Statistics Review**

- Regressions with parameterized sets of functions. e.g.
  - $y = ax^2 + bx + c$  (quadratic)
  - $y = \sum a_i x^i$  (polynomial)
  - $y = Ne^{rx}$ (exponential)

• 
$$y = \frac{1}{1 + e^{-(a+bx)}}$$
 (logistic)





# **Statistics Review**

- Polynomial model of degree 'n'
  - "degrees of freedom" models capacity

![](_page_3_Figure_5.jpeg)

Deep Learning, Goodfellow et. al., MIT Press, http://www.deeplearningbook.org, 2016

![](_page_4_Picture_0.jpeg)

![](_page_4_Picture_1.jpeg)

# **Gradient Decent**

- Searching for minimum
- $\nabla R = \langle R_{\theta_0}, R_{\theta_2}, \dots, R_{\theta_n} \rangle$
- $R(\vec{\theta}_{t+1}) = R(\vec{\theta}_t + \gamma \nabla R)$
- γ: Learning Rate
- Recall, Loss depends on data Expand notation,
  - $R(\vec{\theta}_t; \{(x_i, y_i)\}_n)$
  - Recall R and  $\nabla R$  is a sum over i
- Intuitively, want *R* with ALL DATA .....?  $(R = \sum_{i=1}^{n} [(y_i - f_{\theta_t}(x_i)]^2)$

Fictitious Loss Surface With Gradient Field

![](_page_4_Picture_12.jpeg)

![](_page_5_Picture_0.jpeg)

#### Fictitious Loss Surface With Gradient Field

SORTIUM

#### **Gradient Decent**

![](_page_5_Figure_3.jpeg)

![](_page_6_Picture_0.jpeg)

![](_page_6_Picture_1.jpeg)

### **Stochastic Gradient Decent**

- Recall *R* is a sum over *i*  $(R = \sum_{i=1}^{n} [(y_i f_{\theta_t}(x_i)]^2)]$
- Single training example,  $(x_i, y_i)$ , Sum over only one training example
- $\nabla R_{(x_i, y_i)} = \langle R_{\theta_0}, R_{\theta_2}, \dots, R_{\theta_n} \rangle_{(x_i, y_i)}$
- $R_{(x_i,y_i)}(\vec{\theta}_{t+1}) = R_{(x_i,y_i)}(\vec{\theta}_t + \gamma \nabla R_{(x_i,y_i)})$
- γ: Learning Rate
- Choose next  $(x_{i+1}, y_{i+1})$ , (Shuffled training set)
- SGD with mini batches
- Many training example,  $(x_i, y_i)$ , Sum over many training example
  - Batch Size or Mini Batch Size (This gets ambiguous with distributed training)
- SGD often outperforms traditional GD, want small batches.
  - <u>https://arxiv.org/abs/1609.04836</u>, On Large-Batch Training ... Sharp Minima
  - https://arxiv.org/abs/1711.04325, Extremely Large ... in 15 Minutes

![](_page_7_Picture_0.jpeg)

![](_page_7_Picture_1.jpeg)

# **Neural Networks**

Activation functions
 Logistic

![](_page_7_Figure_4.jpeg)

#### ReLU (Rectified Linear Unit)

![](_page_7_Figure_6.jpeg)

# Arctan $\sigma(x) =$

Softmax

• 
$$g_k(x_1, x_2, ..., x_N) = \frac{e^{x_k}}{\sum e^{x_k}}$$

![](_page_8_Picture_0.jpeg)

![](_page_8_Picture_1.jpeg)

- Parameterized function
  - $Z_M = \sigma(\alpha_{0m} + \alpha_m X)$
  - $T_K = \beta_{0k} + \beta_k Z$
  - $f_K(X) = g_k(T)$
- Linear Transformations with pointwise evaluation of nonlinear function,  $\sigma$
- $\beta_{0i}, \beta_i, \alpha_{0m}, \alpha_m$ 
  - Weights to be optimized

![](_page_8_Figure_9.jpeg)

![](_page_9_Picture_0.jpeg)

![](_page_9_Picture_1.jpeg)

#### Faux Model Example

![](_page_9_Figure_3.jpeg)

![](_page_10_Picture_0.jpeg)

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NCSA

GREAT LAKES CONSORTIUM

#### Distributed Training, data distributed

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![](_page_11_Picture_0.jpeg)

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GREAT LAKES CONSORTIUM

FOR PETASCALE COMPUTATION

NESA

CRAY

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GREAT LAKES CONSORTIUM

FOR PETASCALE COMPUTATION

NCSA

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GREAT LAKES CONSORTIUM

![](_page_13_Figure_2.jpeg)

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Autoregression

$$X_t = c + \sum_{i=1}^p \phi_i B^i X_t + \epsilon_t$$

- Back Shift Operatior: B<sup>i</sup>
  Autocorrelation
  - $R_{XX}(t_1, t_2) = E[X_{t_1}\overline{X_{t_2}}]$
- Other tasks
  - Semantic Labeling

![](_page_14_Figure_8.jpeg)

![](_page_14_Picture_9.jpeg)

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- Few projects use pure RNNs, this example is only for pedagogy
- RNN is a model that is as "deep" as the modeled sequence is long
- LSTM's, Gated recurrent unit,
- No Model Parallel distributed training on the market (June 2019)

![](_page_15_Figure_6.jpeg)