Gradient-Based Learning

BOSTON UNIVERSITY
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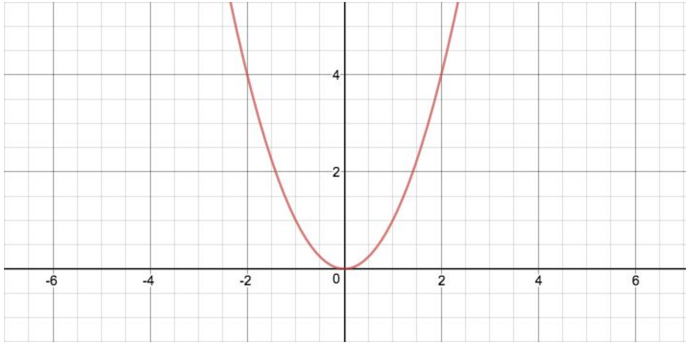
Univariate Functions

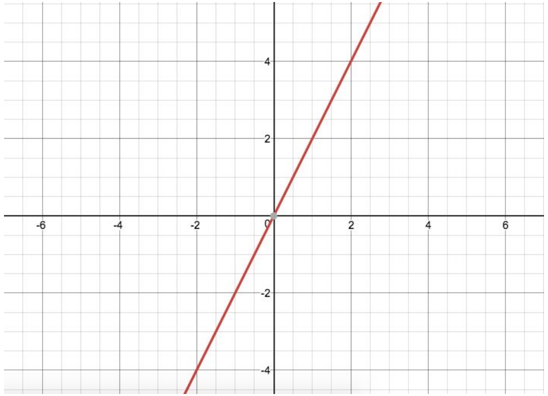
Univariate function

$$f(x) = x^2$$



Derivative

$$\frac{\delta f}{\delta x} = 2\mathrm{x}$$



Multivariate functions

Multivariate function

Function of more than one variable/ **dimension**

$$f(\bar{x}) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 ...$$

Multivariate derivative

Shows us slope of a function in all dimensions

$$\nabla f = \begin{bmatrix} \frac{\delta f}{\delta x_0} \\ \frac{\delta f}{\delta x_1} \\ \vdots \\ \frac{\delta f}{\delta x_n} \end{bmatrix}$$

$$f(x_0, x_1) = 4x_0 + 8x_1$$

$$\nabla f = [4,8]$$

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Linear Equations in PYTORCH

Generate random matrix

```
>> import torch
>> r = torch.randn(2,3)

-0.2220  1.3369 -1.3627
 0.0863  0.8932 -0.6577
[torch.FloatTensor of size 2x3]
```

$$f(\bar{x}) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 \ldots$$

```
>> import torch.nn as nn
>> f = nn.Linear(2,1)
>> [x.data for x in a.parameters()]
[
 0.1685
-0.0136
[torch.FloatTensor of size 2x1]
,
-0.5899
-0.8569
[torch.FloatTensor of size 2]
]
```

weights

bias

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Cost Functions

- Learning algorithms need to measure how wrong it is in order to improve the model
- **Cost function** measures **error** distance between **hypothesis** and **label** (correct answer)
- For example
  - Learning algorithm’s hypothesis: [0.1, 0.2, 0.3]
  - Correct answers: [0.5, 0.8, 0.9]
  - Errors: [0.4, 0.6, 0.6]
  - Least Square Error (LSE): $\frac{1}{2}[(0.1-0.5)^2+(0.2-0.8)^2+(0.3-0.9)^2]$

Different Cost Functions

- Common terms: **cost/ objective/ loss function**
- Tailored for the model
- Common cost functions:

Regression: **Least Square Error**

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

Classification: **Negative Log Likelihood**

$$J(\theta) = \sum_{i=1}^{m}(y^{(i)}log(h_\theta(x^{(i)})) + (1 - y^{(i)})log(1 - h_\theta(x^{(i)})))$$

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Loss Functions in PYTORCH

Negative Log Likelihood

$$J(\theta) = \sum_{i=1}^{m}(y^{(i)}log(h_\theta(x^{(i)})) + (1 - y^{(i)})log(1 - h_\theta(x^{(i)})))$$

```
>> import torch.nn.functional as F
>> from torch.autograd import Variable
>> input = Variable(torch.randn(3, 5))
>> target = autograd.Variable(torch.LongTensor([1, 0, 4]))
>> loss = F.nll_loss(input, target)
Variable containing:
 2.2282
[torch.FloatTensor of size 1]
```

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Optimizing Cost Function

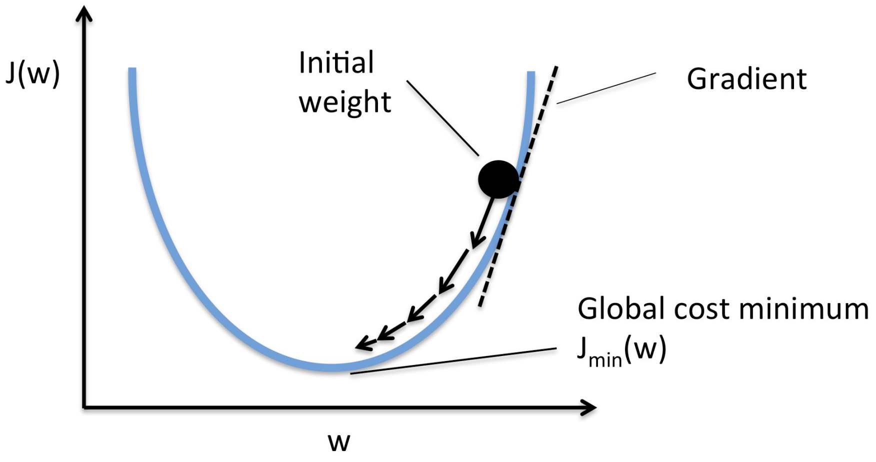
- Goal is to **minimize cost function** J
  - Compute derivative of J w.r.t. parameters θ

$$\nabla J = \frac{\delta J}{\delta \theta}$$

- Consider this simple cost function

$$f(x) = x^2 \quad \longrightarrow \quad \frac{\delta f}{\delta x} = 2\text{x}$$

  - Solve derivative for 0
  - **Convex** functions have single **global minima**
  - Most **cost landscapes** are **non-convex** - contain many **local minima (exponentially many in the number of dimensions)**



https://sebastianraschka.com/faq/docs/closed-form-vs-gd.html

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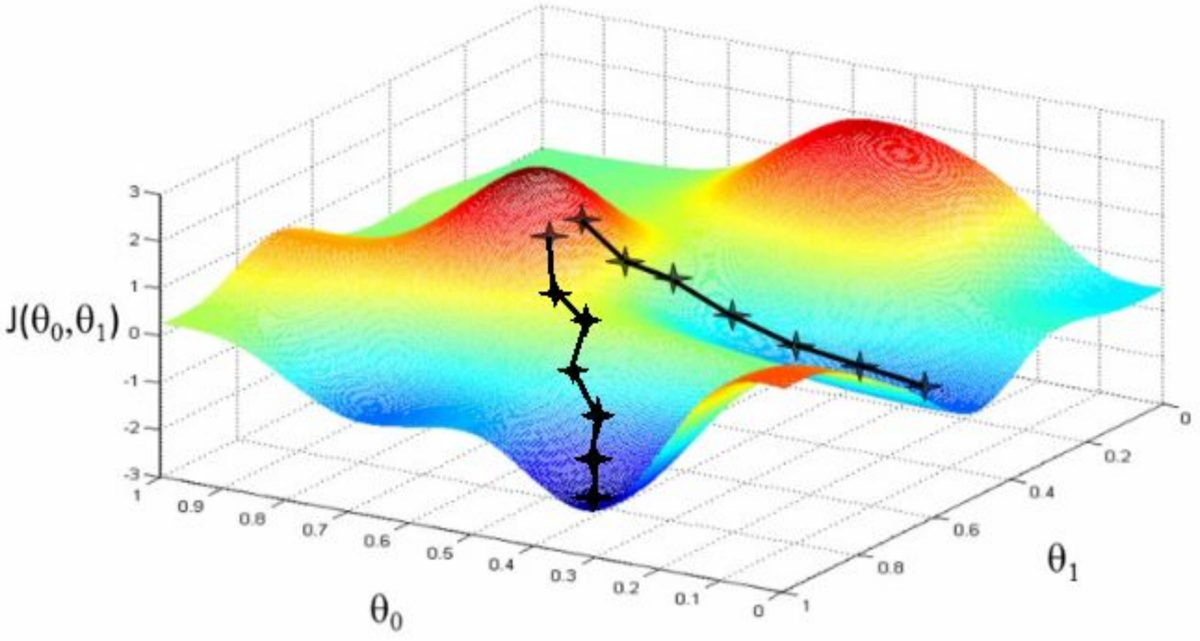
Non-convex Optimization



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Gradient Descent

Scalar learning rate

$$\theta_j := \theta_j - \alpha \overbrace{\frac{\partial}{\partial \theta_j} J(\theta)}^{\text{Also written } \nabla J(\theta)}$$

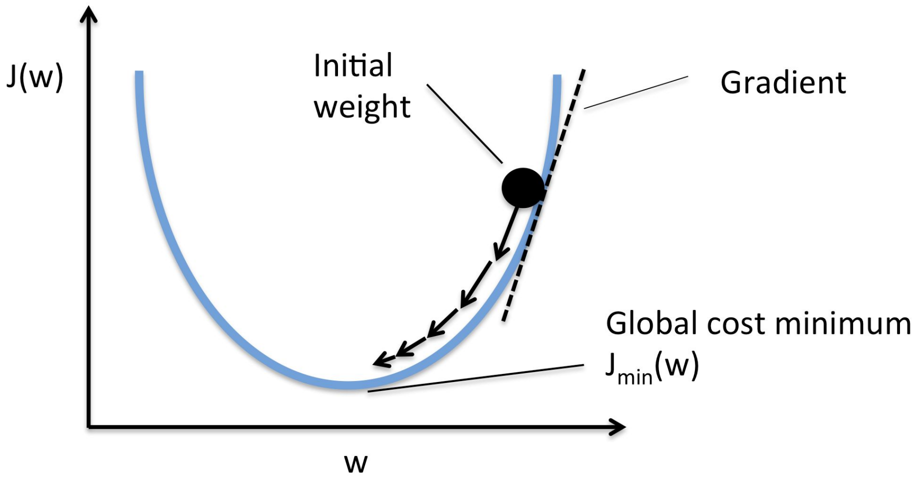
Individual weights

Cost/objective/loss function

Vector of weights

Gradient Descent

- Assumption:
  - Inputs are sampled i.i.d.
- Use gradient to iteratively traverse parameter landscape
- Gradient is direction of steepest descent



https://sebastianraschka.com/faq/docs/closed-form-vs-gd.html

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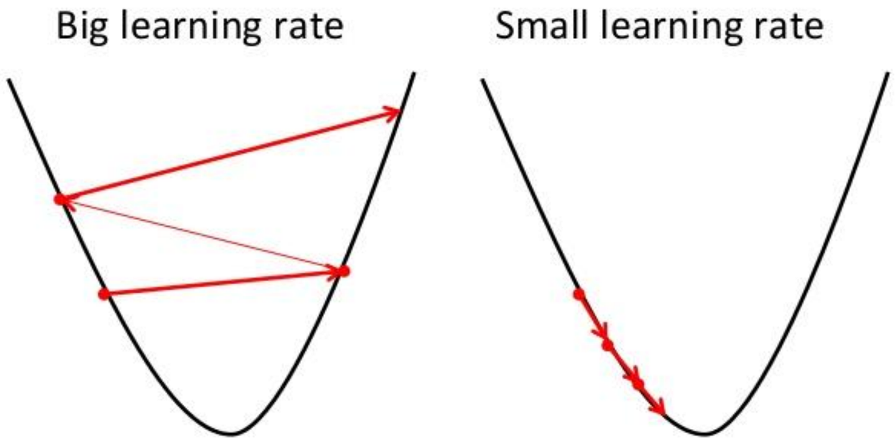
Learning rate

- Gradient points in direct of steepest descent, but does not indicate magnitude of step
- Multiply the learning rate to slow down how fast our network tries to compensate for a given piece of data
- Typical learning rates to try:

  0.1, 0.01, 0.001, 0.0001



Robbins-Monro Conditions

Condition 1:

$$\sum_t \alpha_t = \infty$$

Condition 2:

$$\sum_t \alpha_t^2 < \infty$$

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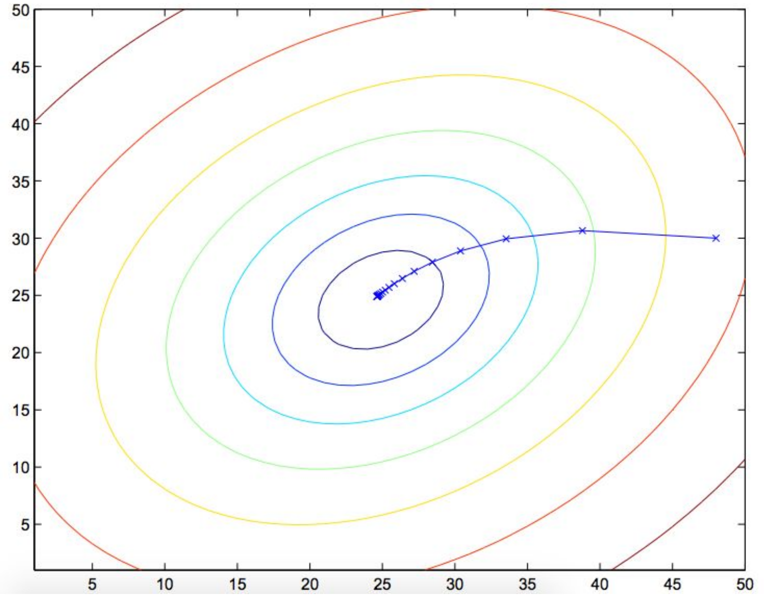
Batch Gradient Descent (GD)

$$Loop\,\{$$

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

$$\}$$



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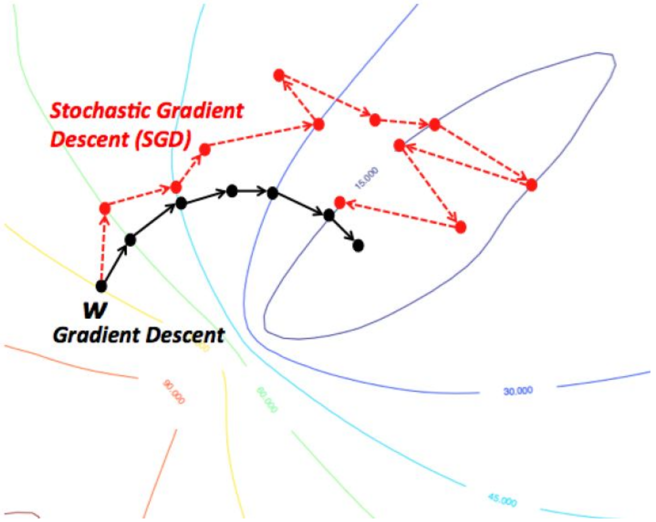
Stochastic Gradient Descent

- Calculate the gradient using one data sample at a time
  - Takes many iterations to go over entire data set
  - Each time the full data set is covered is an “epoch”
- Works better when there are many minima in a complex “manifold”
- Makes for as noisier descent, which can be useful for
  - Noise can be reduced with mini-batch
    - Use 8 or 16 samples at a time
  - Noise can be useful for “saddle points”



http://www.bogotobogo.com/python/scikit-learn/scikit-learn_batch-gradient-descent-versus-stochastic-gradient-descent.php

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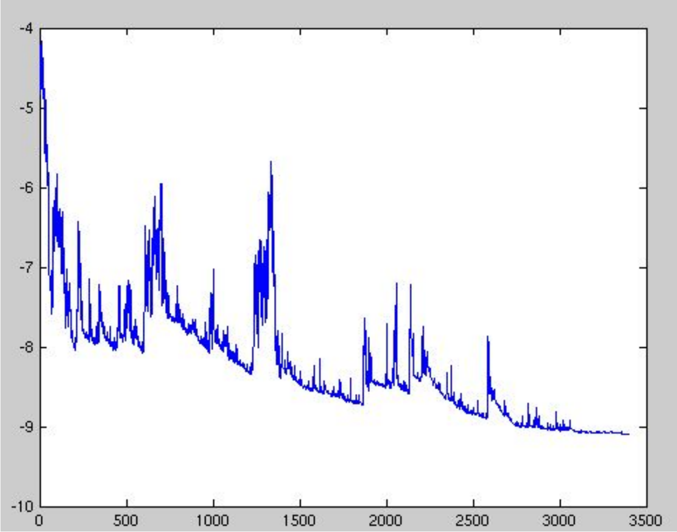
Stochastic Gradient Descent (SGD)

Size of dataset

$$
\begin{aligned}
&Loop\,\{\\
&\quad for\ i = 1\ to\ m\ \{\\
&\qquad \theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)\\
&\quad \}\\
&\}
\end{aligned}
$$



https://upload.wikimedia.org/wikipedia/commons/f/f3/Stogra.png

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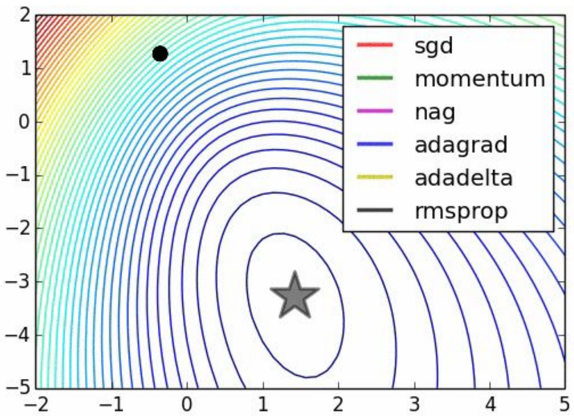
Different types of Gradient Descent

- The concept of gradient descent can be actualized in many different ways. Two popular, and simple, implementations of gradient descent are:
    - Batch gradient descent (which we have been describing so far)
    - Stochastic gradient descent
- A third variety is mini-batch gradient descent
    - Still simple, though more abstract in why it works
    - Between batch and gradient, select batches at a time (ex. 16 out of 100,000)
- For each method, there are multiple algorithms used to optimize the descent calculation



http://blog.hackerearth.com/3-types-gradient-descent-algorithms-small-large-data-sets

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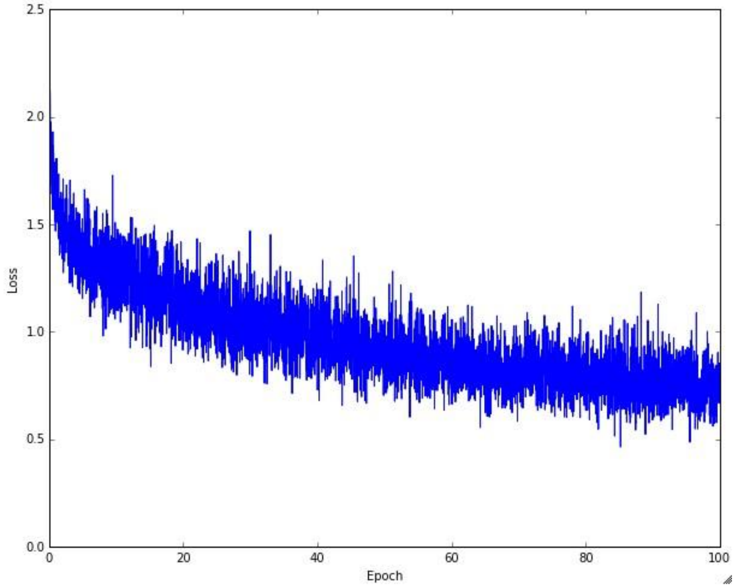
Mini-Batch SGD

Number of mini-batches

$$
\begin{aligned}
&Loop\{\\
&\quad for\ i = 1\ to\ m\ \{\\
&\quad\quad \theta_j := \theta_j - \alpha \frac{1}{|b_i|} \sum_{x \in b_i} \frac{\partial}{\partial \theta_j} J(\theta_j, x)\\
&\quad\}\\
&\}
\end{aligned}
$$

ith mini-batch



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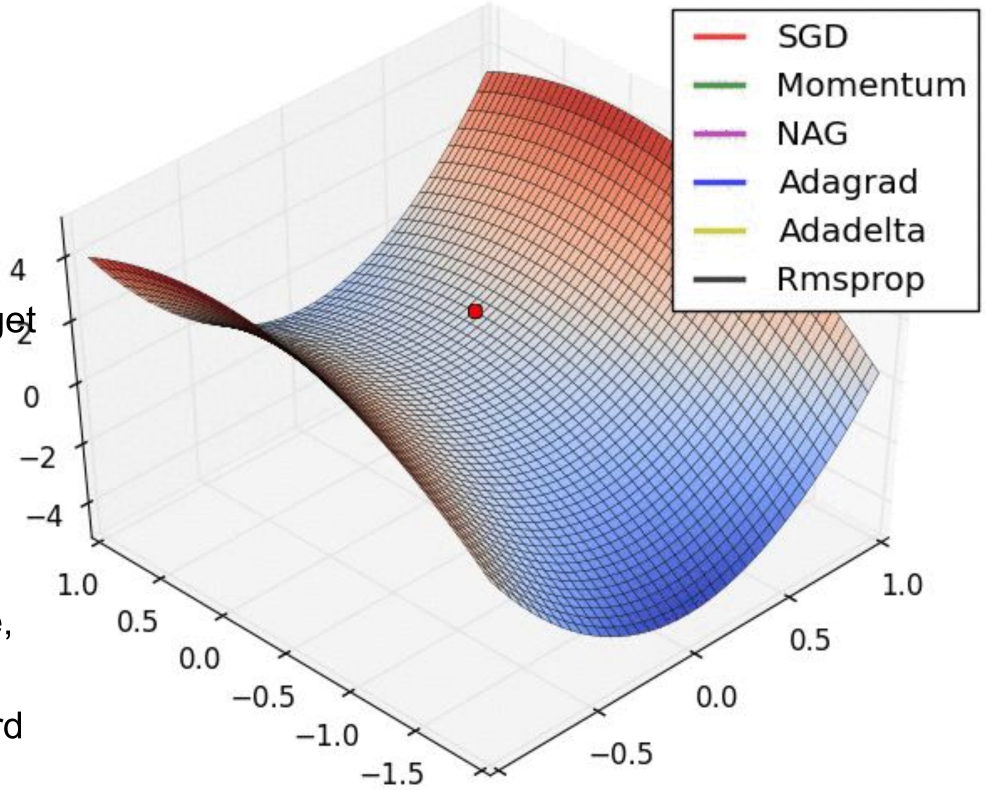
http://cs231n.github.io/neural-networks-3/

Saddle points

- Can be a big issue for gradient descent.
  - If you are right on the saddle, the gradient does not always help you get off
- Can exist above one dimension
- Many solutions to this problem exist
  - A simple one is by just adding noise, you can force the algorithm to randomly “catch on” to the downward slope



http://cs231n.github.io/neural-networks-3/

Backpropagation (BP)

- Method for calculating the error contribution of a single computation unit
    - We can use this information to update weights (parameters), and get closer to a model with less loss
- Neurons (computational units) that contributed more to the error will be changed more by BP
    - Scaled by the learning rate, how much should the weight be adjusted

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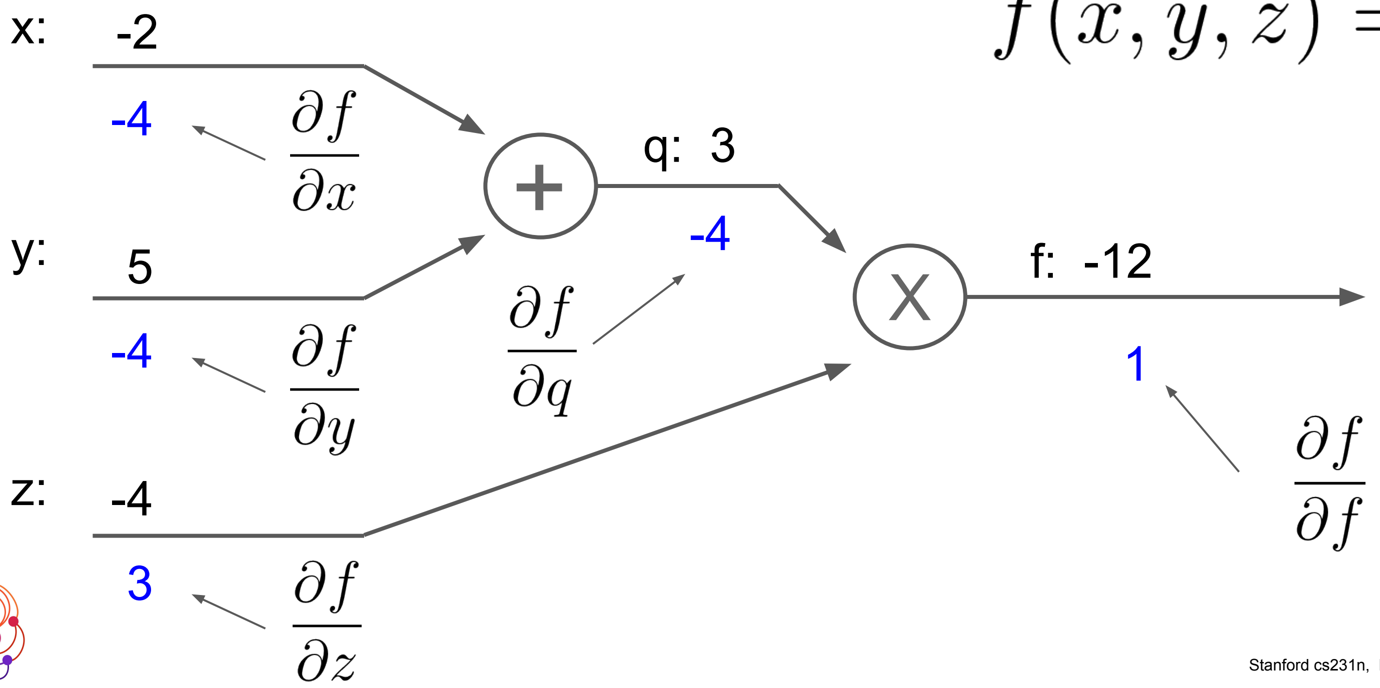
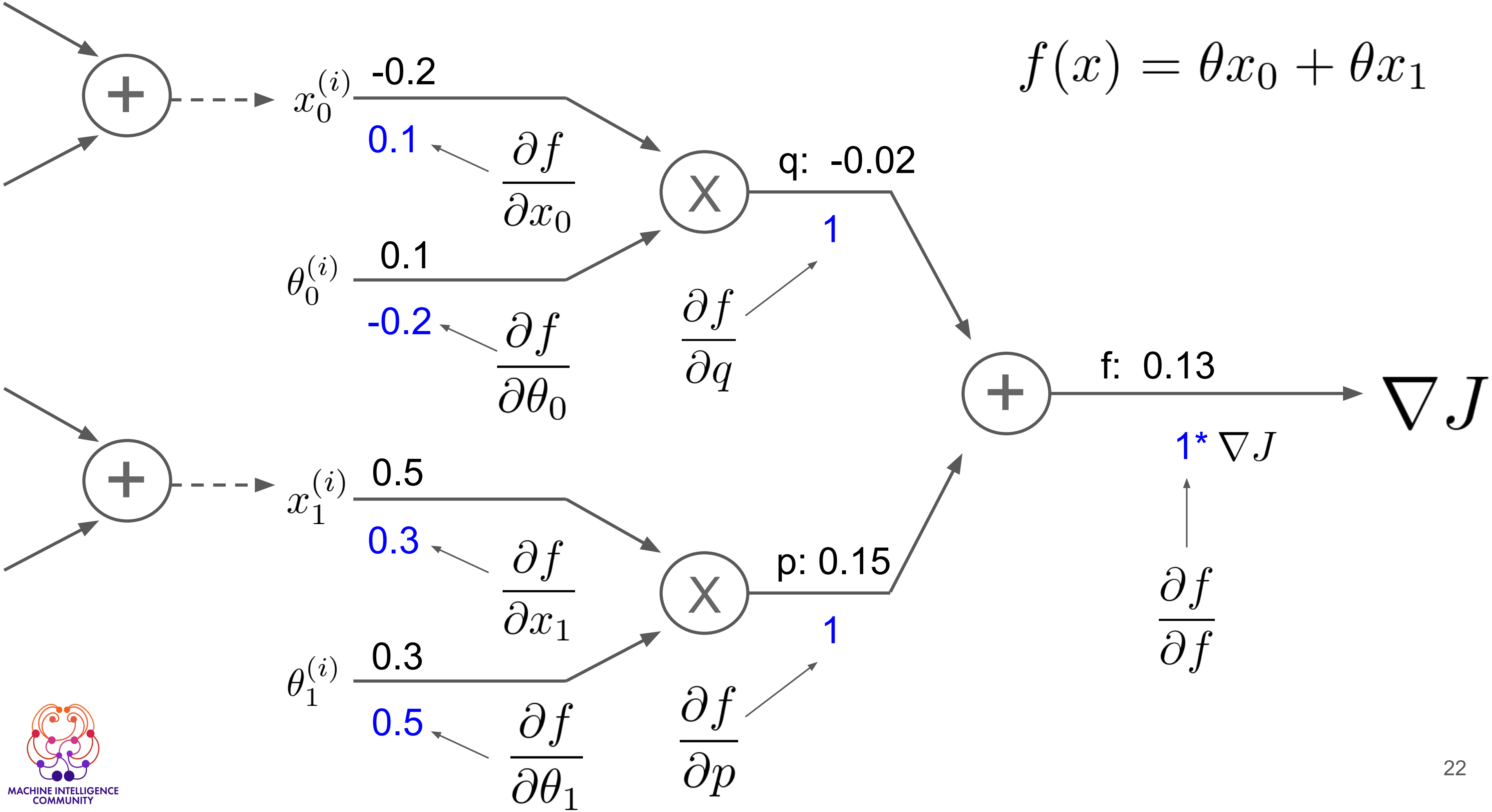
Derivatives of Computation Graph

$$f(x, y, z) = (x + y)z$$



$$f(x) = \theta x_0 + \theta x_1$$



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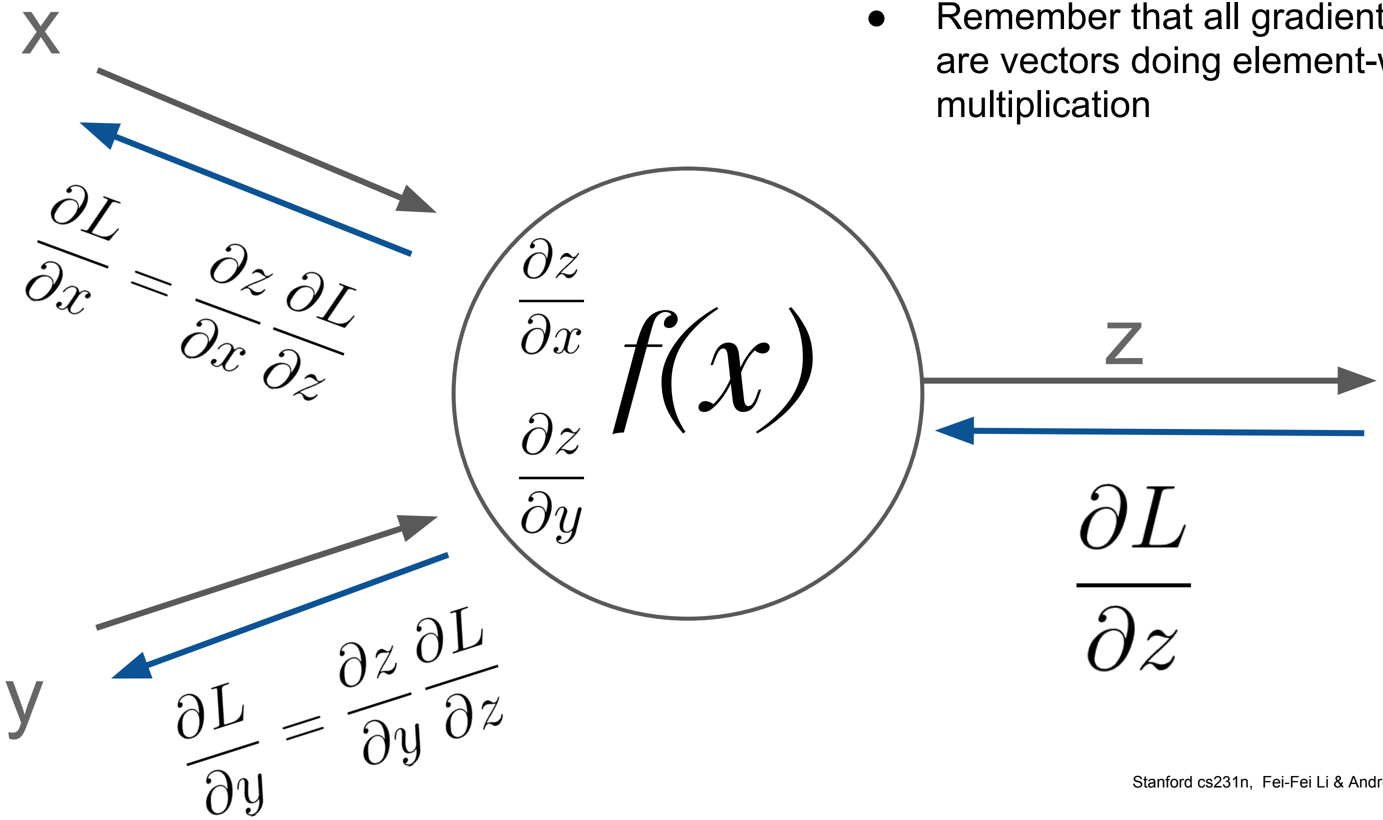
Local Gradient



- Remember that all gradients are vectors doing element-wise multiplication

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Gradient Descent + Backpropagation

- Now, we can adjust a weight based off our gradient descent calculations!
- θ_j can be updated as its old weight minus the change in cost function in respect to itself

Scalar learning rate

$$\theta_j := \theta_j - \alpha \overbrace{\frac{\partial}{\partial \theta_j} J(\theta)}^{\text{Also written } \nabla J(\theta)}$$

Individual weights

Vector of weights

Cost/objective/loss function

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SGD + BP with PYTORCH

```
>> optimizer = torch.optim.SGD(model.parameters(), lr=0.1)
>> optimizer.zero_grad()
>> loss = F.nll_loss(input, target)
>> loss.backward()
>> optimizer.step()
```

1. Define optimizer
2. **Clear local gradients**
3. Compute loss
4. Backpropagate error
5. Apply gradients to parameters

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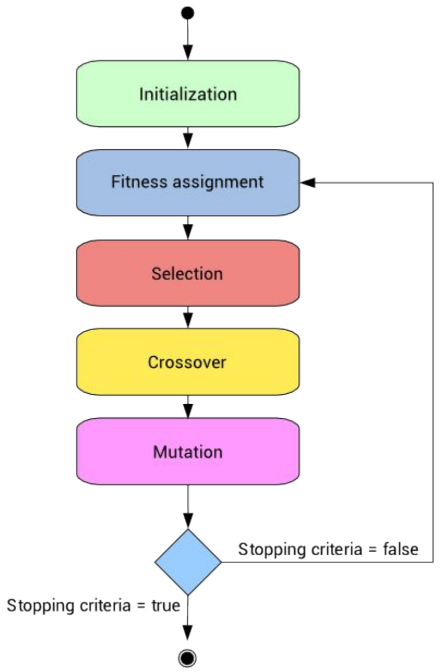
http://pytorch.org/docs/master/optim.html?highlight=sgd#torch.optim.SGD

Anything else besides Gradient Descent?

- Yes, but GD is fairly easy and effective
- Another cool option is using evolution models, or “genetic algorithms”
    - Make random mutations to your model to produce many new generation models
    - Test each one's’ “fitness”
    - Kill off the bad performers, evolve the good ones (feature selection)



https://www.neuraldesigner.com/blog/genetic_algorithms_for_feature_selection

References & Further Reading

[1] Ruder, Sebastian. "An overview of gradient descent optimization algorithms." arXiv preprint arXiv:1609.04747 (2016).

[2] Sun, Xu, et al. "meProp: Sparsified Back Propagation for Accelerated Deep Learning with Reduced Overfitting." arXiv preprint arXiv:1706.06197 (2017).

[3] Kingma, Diederik, and Jimmy Ba. "Adam: A method for stochastic optimization." arXiv preprint arXiv:1412.6980 (2014).

[4] Zeiler, Matthew D. "ADADELTA: an adaptive learning rate method." arXiv preprint arXiv:1212.5701 (2012).

[5] Du, Simon S., et al. "Gradient Descent Can Take Exponential Time to Escape Saddle Points." arXiv preprint arXiv:1705.10412 (2017).

[6] Dean, Jeffrey, et al. "Large scale distributed deep networks." Advances in neural information processing systems. 2012.

[7] Bottou, Léon. "Curiously fast convergence of some stochastic gradient descent algorithms." Proceedings of the symposium on learning and data science, Paris. 2009.

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Upcoming Events

MIC Paper signup: https://goo.gl/iAm6TL
BUMIC Projects signup: https://goo.gl/GmP9oK

MIT MIC reading group:

Paper: Learning from Simulated and Unsupervised Images through Adversarial Training
Location: MIT 56-154 (building 56, room 154)
Date: 9.21.17 Time: 5 PM

BU MIC reading group:

Paper: SimRank Computation on Uncertain Graphs
Location: BU Hariri Seminar Room
Date: 9.22.17 Time: 7 PM

Next workshop:

Location: BU Hariri Seminar Room
Date: 9.26.17 Time: 7 PM

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