Lecture Notes for

Machine Learning in Python

Professor Eric Larson

Optimizing Neural Networks

Class Logistics and Agenda

- Logistics
- Agenda:
  - Finish Town Hall
  - Practical Multi-layer Architectures
  - Programming Examples
- Next Time: More MLPs

Tyler Rablin @Mr_Rablin · 2d

You're not grading assignments.

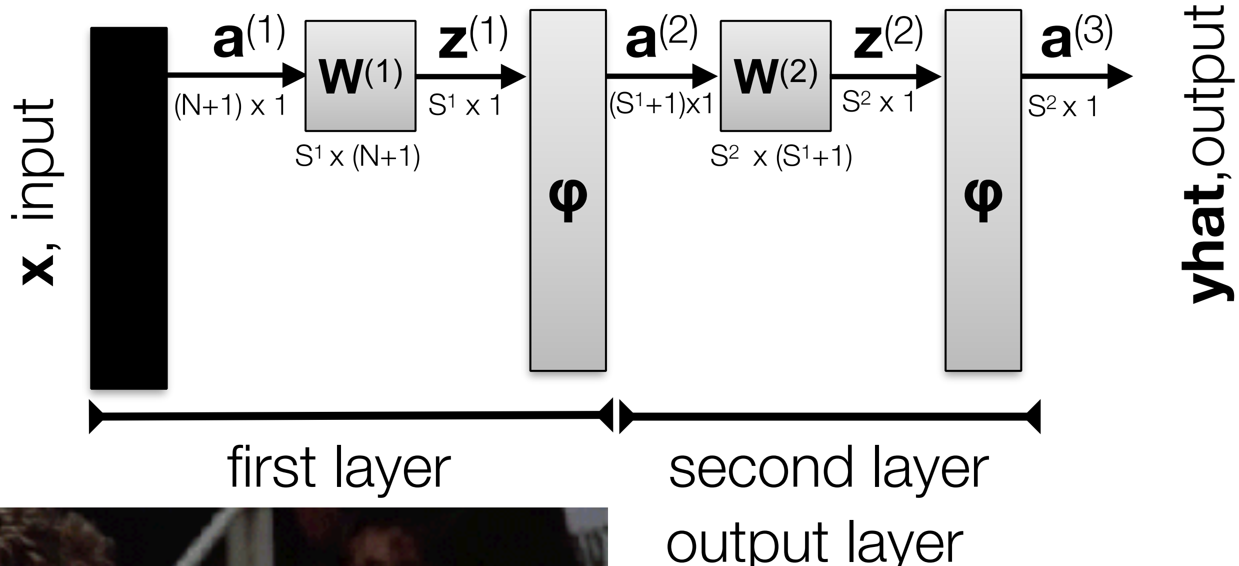
You're collecting evidence to determine student progress and pointing them towards their next steps.

Make the mental switch. It matters.

Town Hall

More Advanced Architectures: MLP

- The multi-layer perceptron (MLP):
  - two layers shown, but could be arbitrarily many layers



each row of **yhat** is no longer independent of the rows in **W** so we cannot optimize using one versus all!!!

$$\mathbf{yhat}^{(i)} = \begin{bmatrix} \varphi\left({}_{row=1}\mathbf{w}^{(2)} \cdot \varphi(\mathbf{W}^{(1)}\mathbf{a}^{(1)})\right) \\ \cdots \\ \varphi\left({}_{row=S}\mathbf{w}^{(2)} \cdot \varphi(\mathbf{W}^{(1)}\mathbf{a}^{(1)})\right) \end{bmatrix}$$

one hot

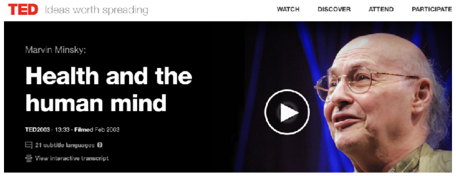
The Rosenblatt-Widrow-Hoff Dilemma

- 1960's: Rosenblatt got into a public academic argument with Marvin Minsky and Seymour Papert

  "Given an elementary α-perceptron, a stimulus world W, and any classification C(W) for which a solution exists; let all stimuli in W occur in any sequence, provided that each stimulus must reoccur in finite time; then beginning from an arbitrary initial state, an error correction procedure will always yield a solution to C(W) in finite time…"

- Minsky and Papert publish limitations paper, 1969:

  "the style of research being done on the perceptron is doomed to failure because of these limitations."



- Widrow and Rosenblatt try to build bigger networks without limitations and fail
  - Neural Networks research **basically stops** for **17 years**
- **Until**: researchers revisit training bigger networks
  - neural networks with multiple layers

More Advanced Architectures: history

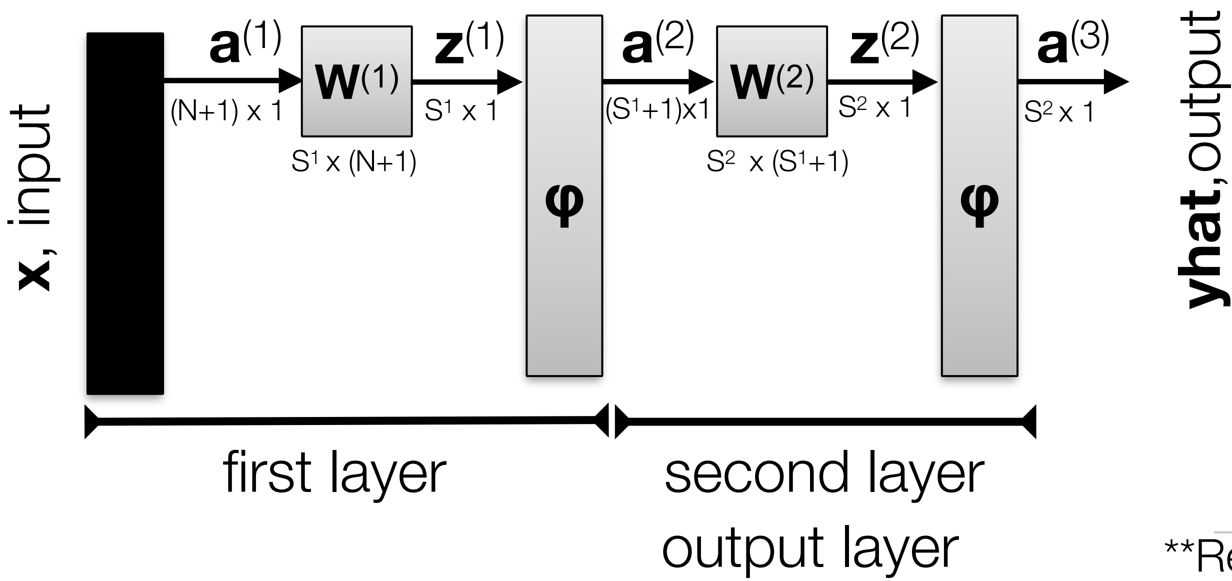
- 1986: *Rumelhart*, *Hinton*, and *Williams* popularize gradient calculation for multi-layer network
    - *actually* introduced by Werbos in 1982
- **difference**: Rumelhart *et al.* validated ideas with a computer
- until this point no one could train a multiple layer network consistently
- algorithm is popularly called **Back-Propagation**
- wins pattern recognition prize in 1993, becomes de-facto machine learning algorithm until: SVMs and Random Forests in ~2004
- would eventually see a resurgence for its ability to train algorithms for Deep Learning applications: **Hinton is widely considered the founder of deep learning**

David Rumelhart

Geoffrey Hinton

Back propagation

- Steps:
  - propagate weights forward
  - calculate gradient at final layer
  - back propagate gradient for each layer
    - via recurrence relation

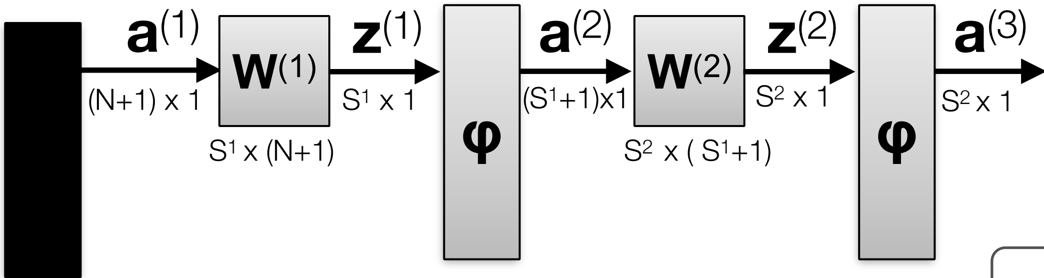


$$J(\mathbf{W}) = \|\mathbf{Y} - \hat{\mathbf{Y}}\|^2$$

$$w_{i,j}^{(l)} \leftarrow w_{i,j}^{(l)} - \eta \frac{\partial J(\mathbf{W})}{\partial w_{i,j}^{(l)}}$$

**Recall from Flipped Assignment!

Back Propagation Summary



1. Forward propagate to get **Z**, **A**
2. Get final layer gradient
3. Back propagate sensitivities
4. Update each $\mathbf{W}^{(l)}$

$$\mathbf{V}^{(2)} = -2(\mathbf{Y} - \mathbf{A}^{(3)}) * \mathbf{A}^{(3)} * (1 - \mathbf{A}^{(3)})$$

$$\nabla^{(2)} = \mathbf{V}^{(2)} \cdot [\mathbf{A}^{(2)}]^T$$

$$\mathbf{V}^{(1)} = \mathbf{A}^{(2)} * (1 - \mathbf{A}^{(2)}) * [\mathbf{W}^{(2)}]^T \cdot \mathbf{V}^{(2)}$$

$$\nabla^{(1)} = \mathbf{V}^{(1)} \cdot [\mathbf{A}^{(1)}]^T$$

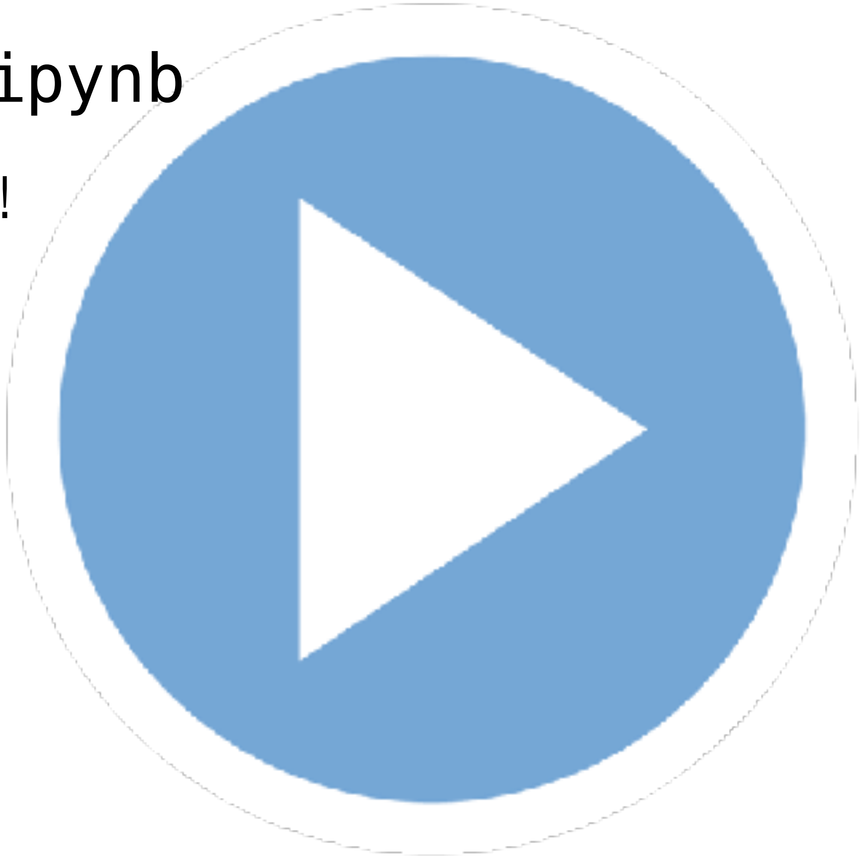
$$\mathbf{W}^{(l)} \leftarrow \mathbf{W}^{(l)} - \eta \nabla^{(l)}$$

Where is the problem of **vanishing gradients** introduced?

**Recall from Flipped Assignment!

07. MLP Neural Networks.ipynb

same as Flipped Assignment!
with regularization
and vectorization



Problems with Advanced Architectures

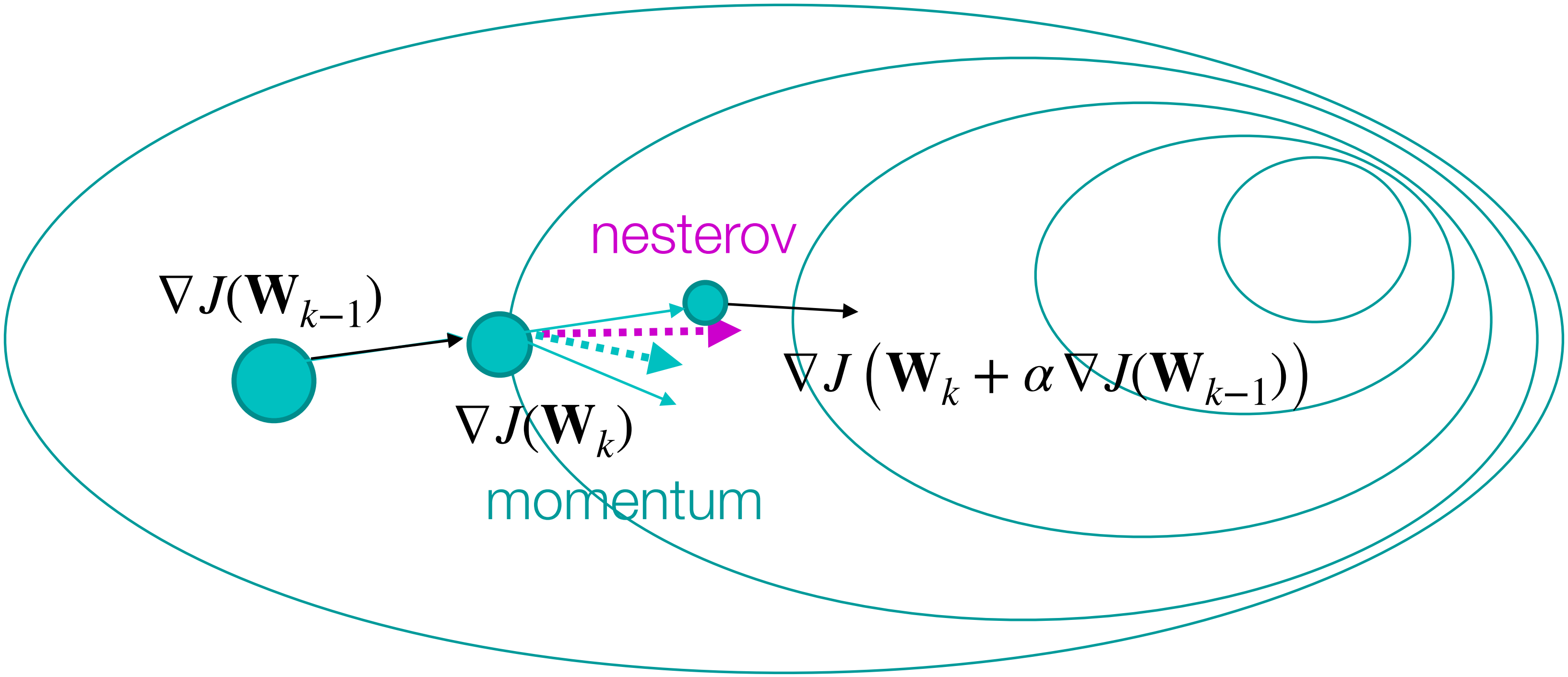
- Numerous weights to find gradient update
  - minimize number of instances
  - **solution**: mini-batch
- **new problem**: mini-batch gradient can be erratic
  - **solution**: momentum
    - use previous update in current update

Common Adaptive Strategies

$$\mathbf{W}_{k+1} = \mathbf{W}_k - \rho_k$$

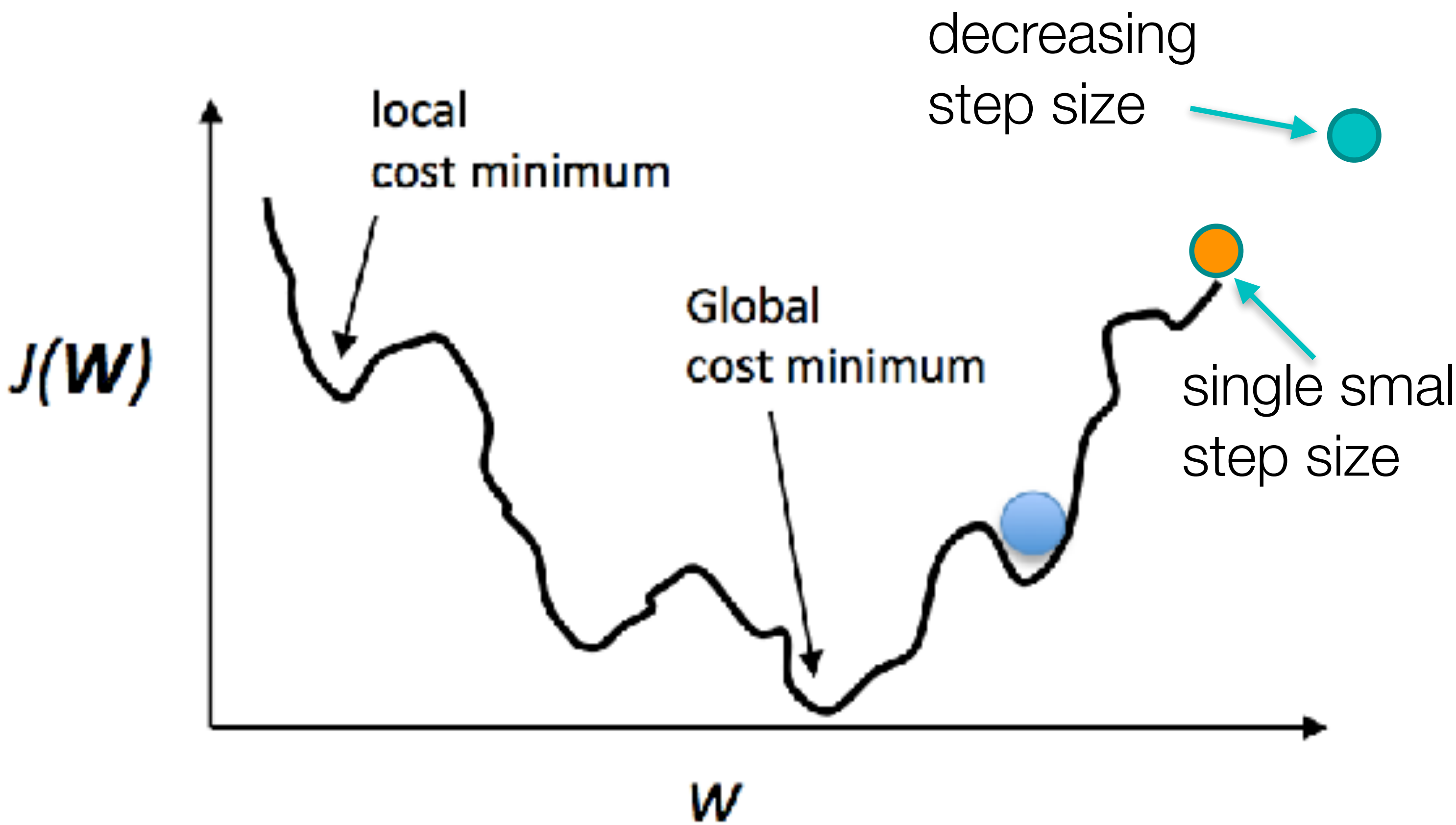
- Momentum $\rho_k = \alpha \nabla J(\mathbf{W}_k) + \beta \nabla J(\mathbf{W}_{k-1})$

- Nesterov's Accelerated Gradient $\rho_k = \underbrace{\beta \nabla J\left(\mathbf{W}_k + \alpha \nabla J(\mathbf{W}_{k-1})\right)}_{\text{step twice}} + \alpha \nabla J(\mathbf{W}_{k-1})$



Adaptive Strategy: Cooling

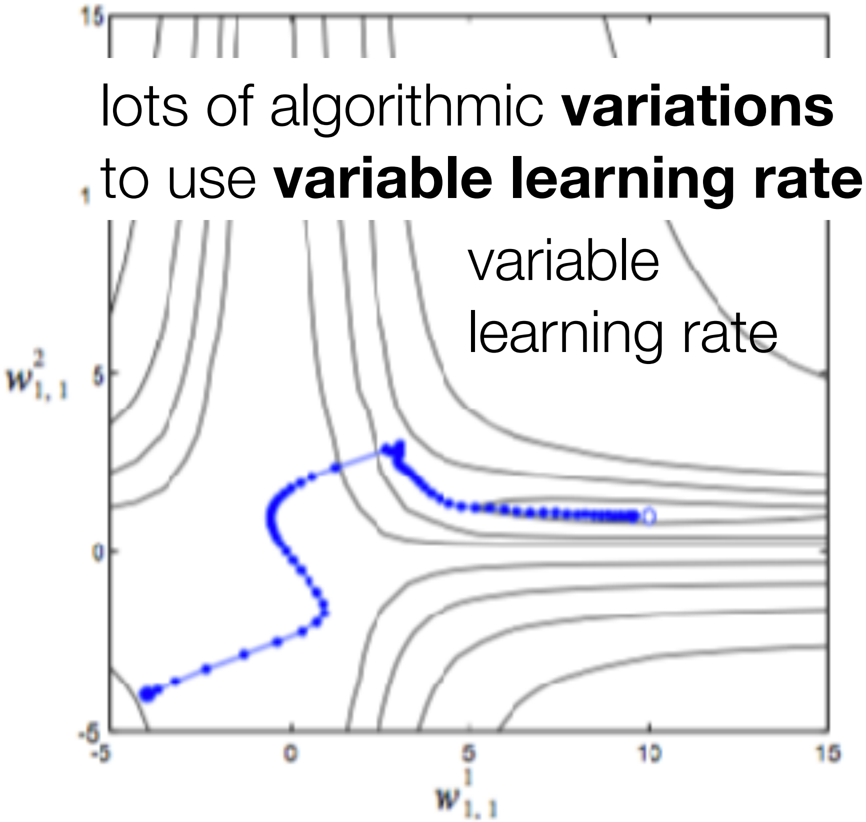
- Space is no longer convex
    - **One solution**:
        - start with large step size
        - “cool down” by decreasing step size for higher iterations

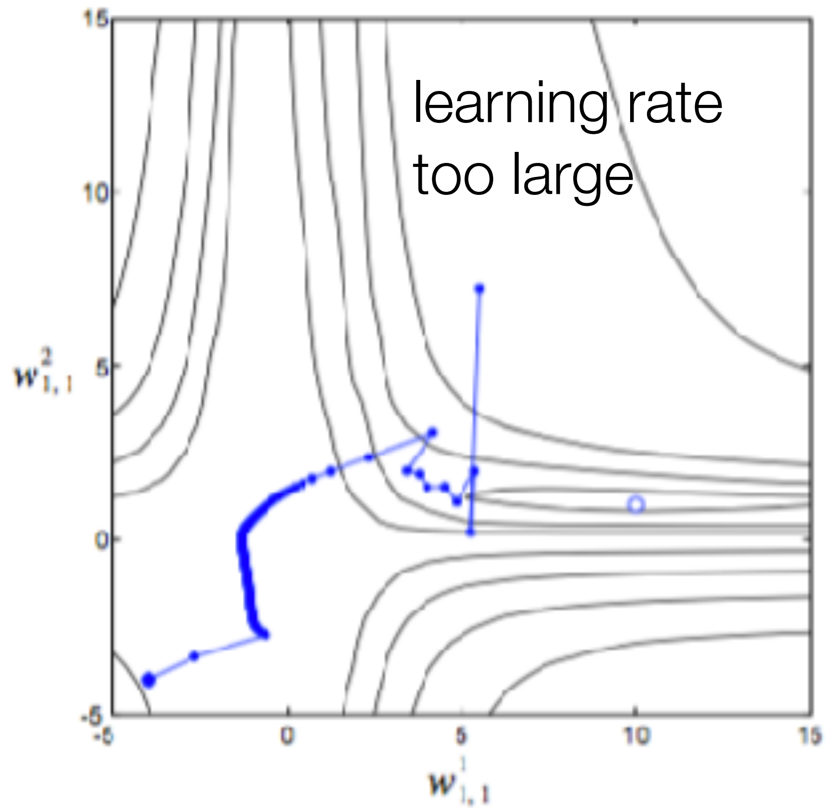


Another Adaptive Strategy $\mathbf{W}_{k+1} = \mathbf{W}_k - \eta^k \cdot \rho_k$

- Space is no longer convex
  - **another solution**:
    - start with arbitrary step size
    - only decrease when successive iterations do not decrease cost

lots of algorithmic **variations** to use **variable learning rate**





Neural Network Design, Hagan, Demuth, Beale, and De Jesus

Demo

`07. MLP Neural Networks.ipynb`

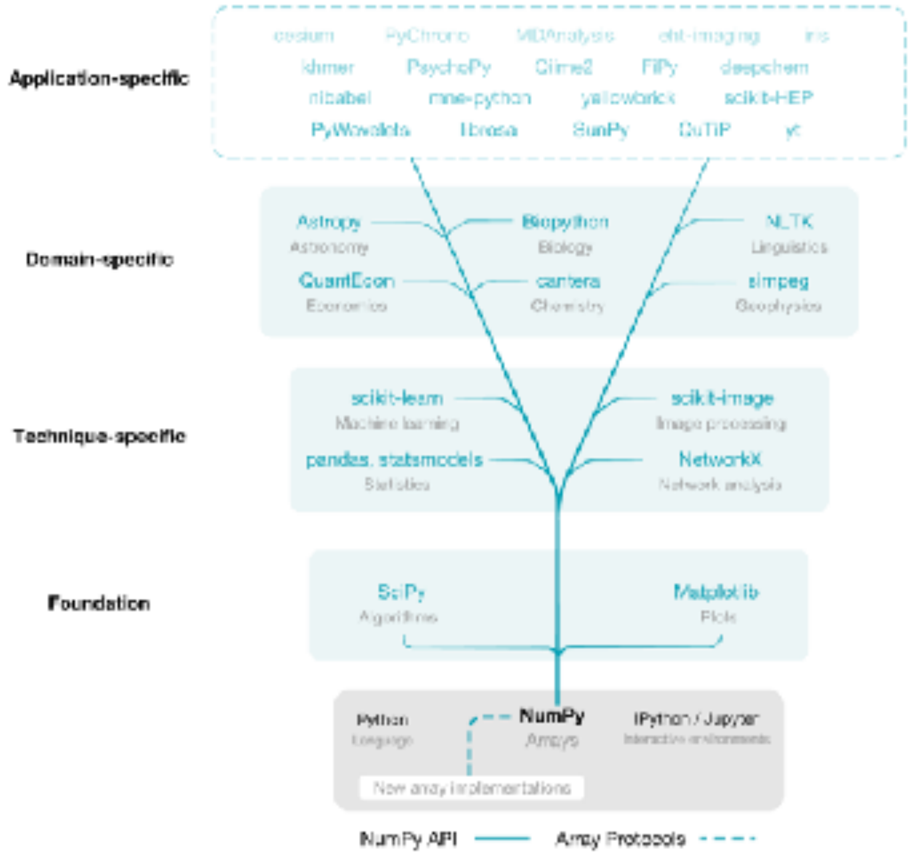
comparison:

- mini-batch
  - momentum
  - adaptive learning
- L-BFGS

Adaptive Optimization

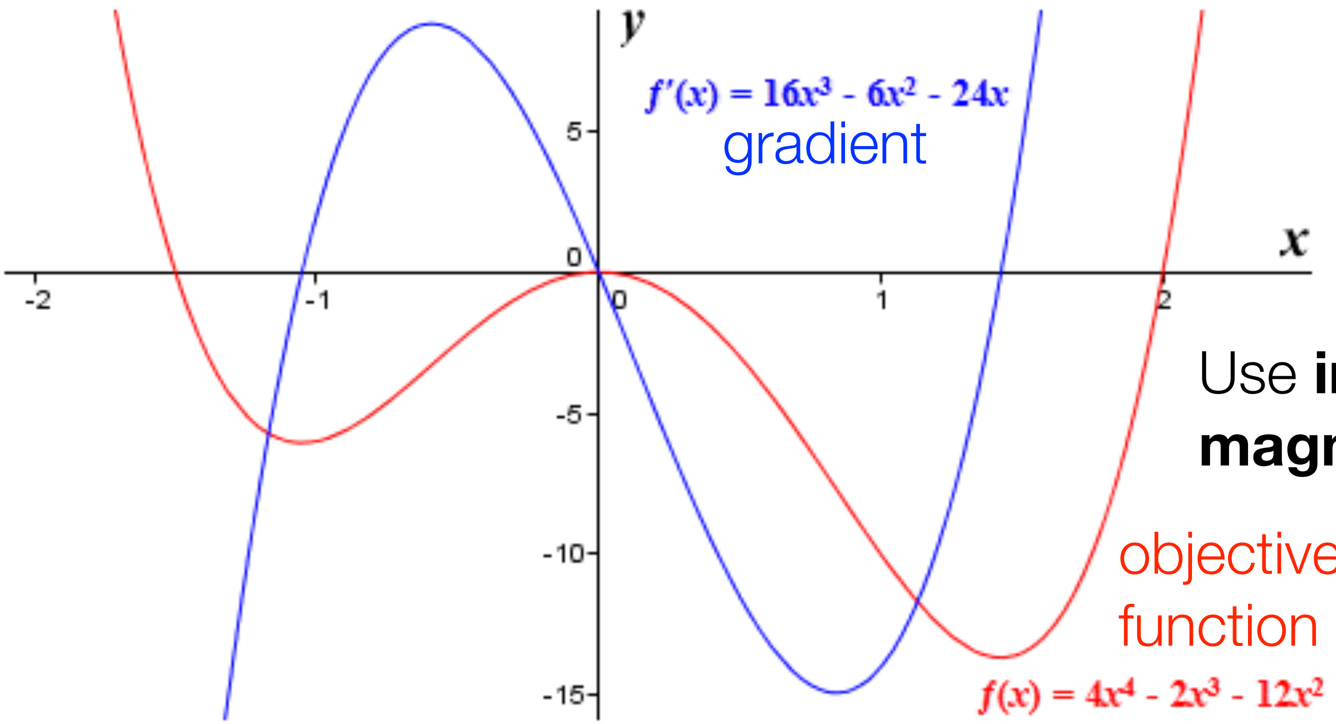
Fig. 2: NumPy is the base of the scientific Python ecosystem.

From: Array programming with NumPy



Be adaptive based on Gradient Magnitude?

- Decelerate down regions that are steep
- Accelerate on plateaus



Use **inverse** of **magnitude** of **gradient**!

Also **accumulate inverse** to be robust to **abrupt changes** in **steepness**…

http://www.technologyuk.net/mathematics/differential-calculus/higher-derivatives.shtml

Common Adaptive Strategies $\mathbf{W}_{k+1} = \mathbf{W}_k - \rho_k$

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- Nesterov's Accelerated Gradient $$\rho_k = \underbrace{\beta \nabla J \left(\mathbf{W}_k + \alpha \nabla J(\mathbf{W}_{k-1})\right)}_{\text{step twice}} + \alpha \nabla J(\mathbf{W}_{k-1})$$

- AdaGrad $$\rho_k = \frac{\eta}{\sqrt{G_k + \epsilon}} \odot \nabla J(\mathbf{W}_k)$$ where $$G_k = G_{k-1} + \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$$

all operations are per element

- RMSProp $$\rho_k = \frac{\eta}{\sqrt{V_k + \epsilon}} \odot \nabla J(\mathbf{W}_k)$$ $$G_k = \nabla J(\mathbf{W}_k) \odot \nabla J(\mathbf{W}_k)$$ $$V_k = \gamma \cdot V_{k-1} + (1-\gamma) \cdot G_k$$

all operations are per element

- AdaDelta $$\rho_k = \frac{\sqrt{M_k + \epsilon}}{\sqrt{V_k + \epsilon}} \odot \nabla J(\mathbf{W}_k)$$ $$M_k = \gamma \cdot M_k + (1-\gamma) \cdot \nabla J(\mathbf{W}_k)$$

all operations are per element

- AdaM G updates with decaying momentum of J and J^2

- NAdaM same as Adam, but with nesterov's acceleration

None of these are **"one-size-fits-all"** because the space of neural network **optimization varies** by problem, ADAM is **popular** but **not a panacea**

Adaptive Momentum

All operations are element wise:

$$\beta_1 = 0.9,\ \beta_2 = 0.999,\ \eta = 0.001,\ \epsilon = 10^{-8}$$

$$k = 0,\ \mathbf{M}_0 = \mathbf{0},\ \mathbf{V}_0 = \mathbf{0}$$

Published as a conference paper at ICLR 2015

ADAM: A METHOD FOR STOCHASTIC OPTIMIZATION

Diederik P. Kingma* University of Amsterdam, OpenAI
Jimmy Lei Ba* University of Toronto

For each epoch:

update epoch $k \leftarrow k + 1$

get gradient $\mathbf{G}_k \leftarrow \nabla J(\mathbf{W}_k)$

accumulated gradient $\mathbf{M}_k \leftarrow \beta_1 \cdot \mathbf{M}_{k-1} + (1 - \beta_1) \cdot \mathbf{G}_k$

accumulated squared gradient $\mathbf{V}_k \leftarrow \beta_2 \cdot \mathbf{V}_{k-1} + (1 - \beta_2) \cdot \mathbf{G}_k \odot \mathbf{G}_k$

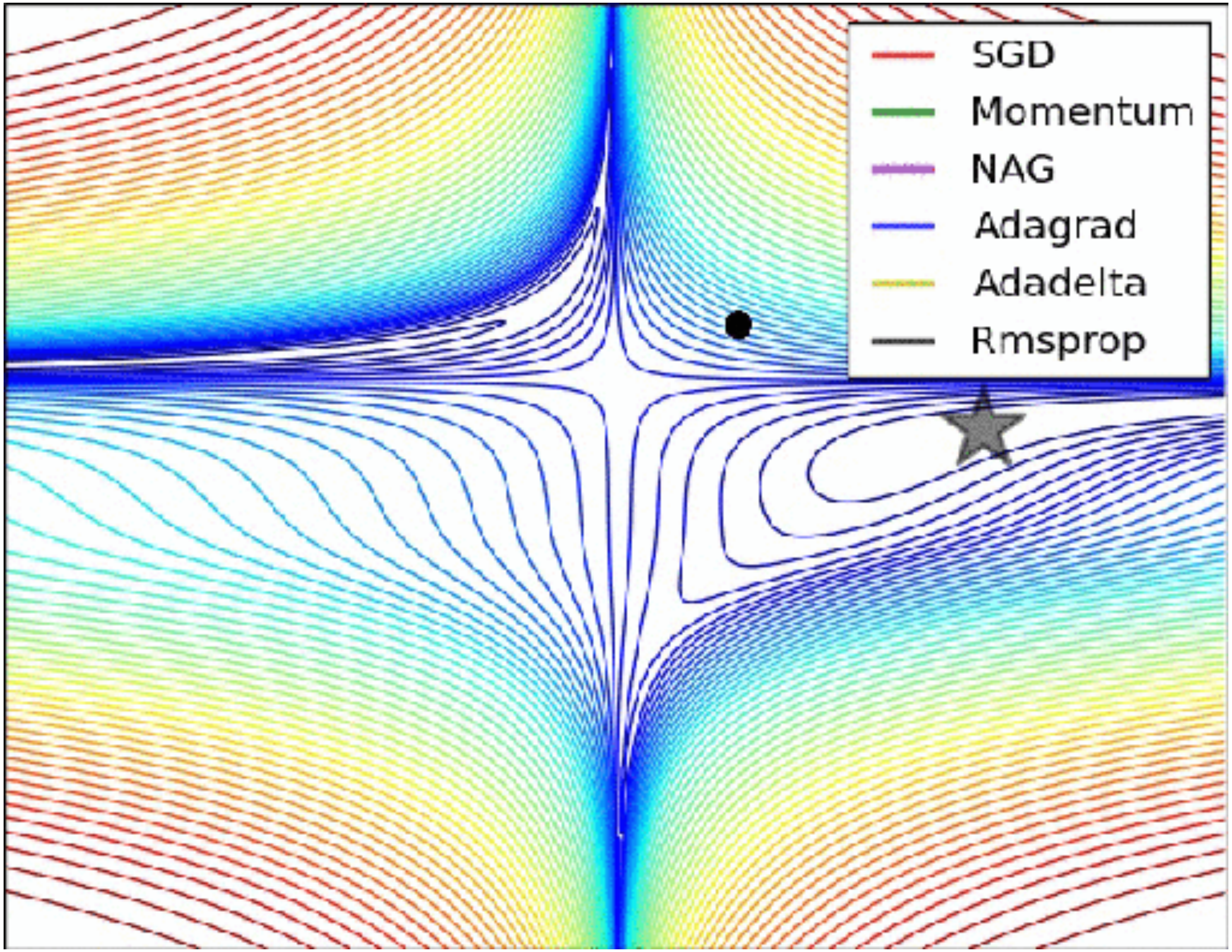
boost moments magnitudes (notice k in exponent)

$$\hat{\mathbf{M}}_k \leftarrow \frac{\mathbf{M}_k}{(1 - [\beta_1]^k)} \qquad \hat{\mathbf{V}}_k \leftarrow \frac{\mathbf{V}_k}{(1 - [\beta_2]^k)}$$

update gradient, normalized by second moment similar to AdaDelta

$$\mathbf{W}_k \leftarrow \mathbf{W}_{k-1} - \eta \cdot \frac{\hat{\mathbf{M}}_k}{\sqrt{\hat{\mathbf{V}}_k + \epsilon}}$$

Visualization of Optimization



https://ruder.io/optimizing-gradient-descent/