The Math Behind Neural Networks

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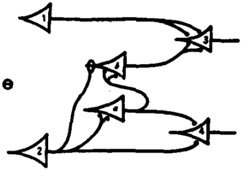
Note: I’ve ripped off all images in this presentation.

The Brain and the Machine

1942 A Logical Calculus of Ideas Immanent in Nervous Activity



- McCulloch & Pitts
- Neurons + Synapses

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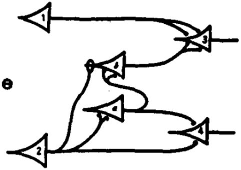

- McCulloch & Pitts
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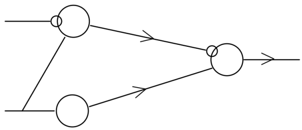
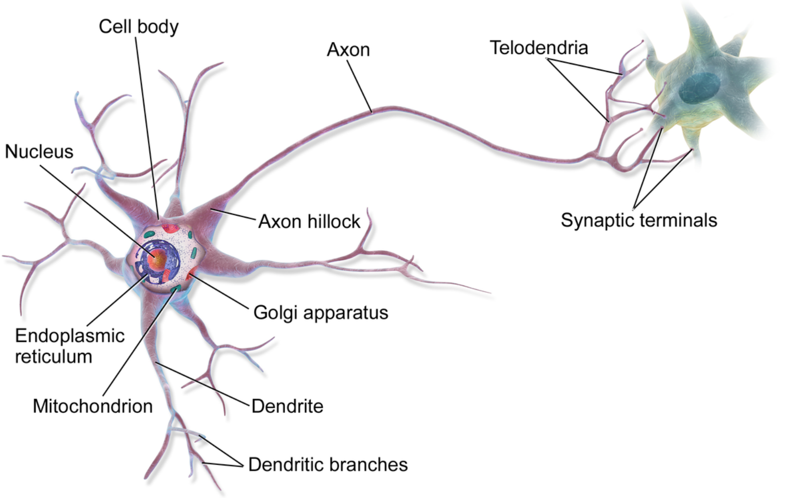
1945 First Draft of a Report on the EDVAC

FIGURE 2



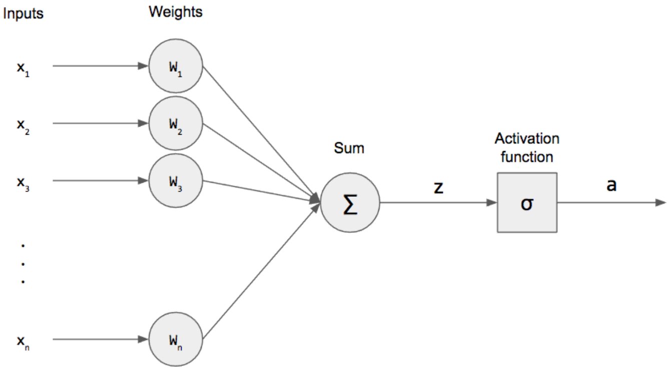
- von Neumann
- Defines E-Elements

Actual Neuron

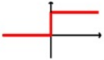
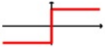


Perceptron

1958 The perceptron: A probabilistic model for information storage and organization in the brain.



Activation Functions

Activation Function	Equation	Example	1D Graph
Linear	$\phi(z) = z$	Adaline, linear regression	
Unit Step (Heaviside Function)	$\phi(z) = \begin{cases} 0 & z < 0 \\ 0.5 & z = 0 \\ 1 & z > 0 \end{cases}$	Perceptron variant	
Sign (signum)	$\phi(z)= \begin{cases} -1 & z < 0 \\ 0 & z = 0 \\ 1 & z > 0 \end{cases}$	Perceptron variant	
Piece-wise Linear	$\phi(z)= \begin{cases} 0 & z \leq -\frac{1}{2} \\ z + \frac{1}{2} & -\frac{1}{2} \leq z \leq \frac{1}{2} \\ 1 & z \geq \frac{1}{2} \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z)= \dfrac{1}{1 + e^{-z}}$	Logistic regression, Multilayer NN	
Hyperbolic Tangent (tanh)	$\phi(z)= \dfrac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$	Multilayer NN, RNNs	
ReLU	$\phi(z)= \begin{cases} 0 & z < 0 \\ z & z > 0 \end{cases}$	Multilayer NN, CNNs	

Perceptron Inference

- Notation

x : input data vector of size n

w : weight vector of size n

α : activation function

o : prediction output

- Inference

$$z = \sum_{i=1}^{n} x_i w_i$$

$$o = \alpha(z)$$

Basic Perceptron Training

- Notation

  t : target label in $\{0, 1\}$

  o : prediction output

  η : learning rate

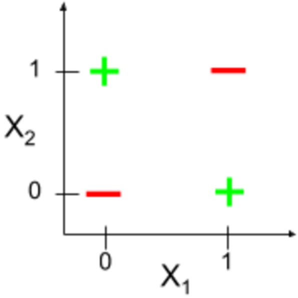
- Update Step: for all (x, t)

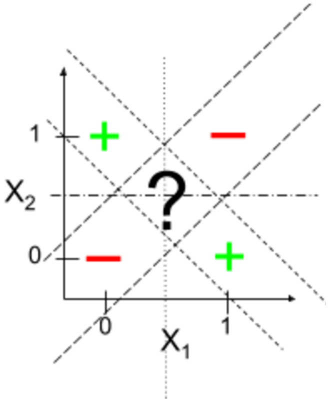
$$w = w + \Delta w$$

$$\Delta w = \eta \, x \, (t - o)$$

- Converges if $x \in X$ is linearly separable

Issue with Basic Training





Perceptron Training with Gradient Descent

- Notation

  $\mathscr{L}(X, w, t)$: loss function

- Update

$$\Delta w = -\eta \frac{\partial \mathscr{L}}{\partial w}$$

Perceptron GD Example

- Mean Squared Error

$$\mathscr{L}_{MSE}(X, w, t) = \frac{1}{2}\,\mathbb{E}_{j=1}^{d}(t_j - o_j)^2$$

- Sigmoid Activation

$$\alpha(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$

Gradient of MSE

- Gradient Contribution for a single (x, t)

$$\frac{\partial \mathscr{L}}{\partial w_i} = \frac{\partial \mathscr{L}}{\partial o} \frac{\partial o}{\partial z} \frac{\partial z}{\partial w_i}$$

Gradient of MSE

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$$\frac{\partial z}{\partial w_i} = \frac{\partial}{\partial w_i} \sum_{j=1}^{n} w_j x_j = x_i$$

Gradient of MSE : Put it All Together

- Gradient Contribution for a single (x, t)

$$\begin{aligned}\frac{\partial \mathscr{L}}{\partial w_i} &= \frac{\partial \mathscr{L}}{\partial o}\frac{\partial o}{\partial z}\frac{\partial z}{\partial w_i} \\ &= -(t-o)\sigma(z)(1-\sigma(z))x_i \\ &= -(t-o)(o-o^2)x_i\end{aligned}$$

- Update Weights

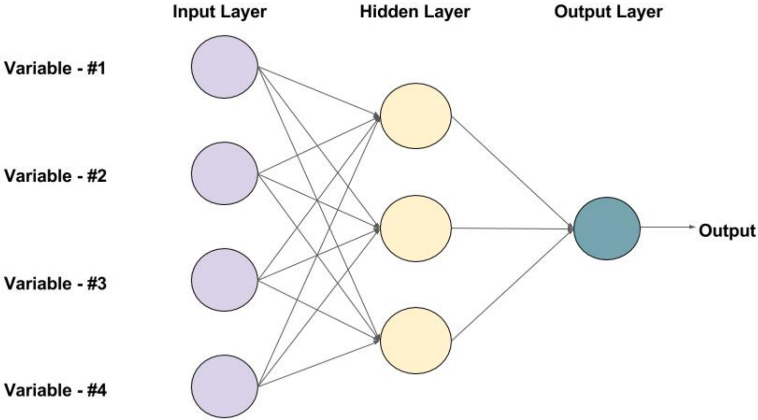
$$\Delta w_i = -\eta\frac{\partial \mathscr{L}}{\partial w_i} = \eta\,\mathbb{E}_{x\in X}(t-o)(o-o^2)x_i$$

Gradient of MSE : Implications

$$\Delta w_i = \eta \, \mathbb{E}_{x \in X} (t - o)(o - o^2) x_i$$

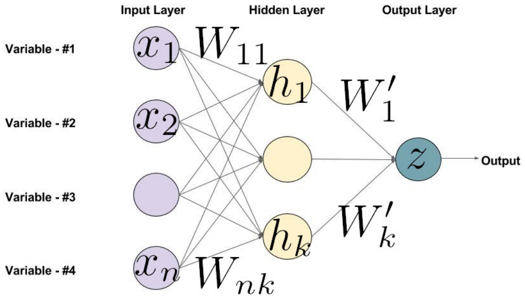
- Weight update is largest when $o = 0.5$, vanishes elsewhere.
- Weight update is proportional to x_i.
- Weight does NOT update if $t = o$.

Feed-Forward Neural Network



An example of a Feed-forward Neural Network with one hidden layer (with 3 neurons)

Feed-Forward Neural Network : Notation



An example of a Feed-forward Neural Network with one hidden layer (with 3 neurons)

$$h_j = \sum_{i=1}^{n} W_{ij} x_i + b_j \qquad z = \sum_{j=1}^{k} W'_j o_j^{(h)} + b'$$

$$o_j^{(h)} = h_j \qquad o = \sigma(z)$$

Back Propagation

- Weight Update:

$$\Delta W = -\eta \frac{\partial \mathscr{L}}{\partial W}$$

Back Propagation

- Weight Update:

$$\Delta W = -\eta \frac{\partial \mathscr{L}}{\partial W}$$

- Derivative in last layer (look familiar):

$$\frac{\partial \mathscr{L}}{\partial W'_j} = \frac{\partial \mathscr{L}}{\partial o} \frac{\partial o}{\partial z} \frac{\partial z}{\partial W'_j}$$

Back Propagation

- Weight Update:

$$\Delta W = -\eta \frac{\partial \mathscr{L}}{\partial W}$$

- Derivative in last layer (look familiar):

$$\frac{\partial \mathscr{L}}{\partial W'_j} = \frac{\partial \mathscr{L}}{\partial o} \frac{\partial o}{\partial z} \frac{\partial z}{\partial W'_j}$$

- Derivative in hidden layer:

$$\frac{\partial \mathscr{L}}{\partial W_{ij}} = \frac{\partial \mathscr{L}}{\partial o} \frac{\partial o}{\partial z} \frac{\partial z}{\partial o_j^{(h)}} \frac{\partial o_j^{(h)}}{\partial h_j} \frac{\partial h_j}{\partial W_{ij}}$$

Gradient at Hidden Layer

- Gradient contribution for a single (x, t) on weight W_{ij}.

$$\frac{\partial \mathscr{L}}{\partial W_{ij}} = \frac{\partial \mathscr{L}}{\partial o} \frac{\partial o}{\partial z} \frac{\partial z}{\partial o_j^{(h)}} \frac{\partial o_j^{(h)}}{\partial h_j} \frac{\partial h_j}{\partial W_{ij}}$$

Gradient at Hidden Layer

- Gradient contribution for a single (x, t) on weight W_{ij}.

$$\frac{\partial \mathcal{L}}{\partial W_{ij}} = \frac{\partial \mathcal{L}}{\partial o}\frac{\partial o}{\partial z}\frac{\partial z}{\partial o_j^{(h)}}\frac{\partial o_j^{(h)}}{\partial h_j}\frac{\partial h_j}{\partial W_{ij}}$$

- Same as before

$$\frac{\partial \mathcal{L}}{\partial o}\frac{\partial o}{\partial z} = -(t-o)(o-o^2)$$

- Hidden Propagation

$$\frac{\partial z}{\partial o_j^{(h)}} = W'_j \quad \frac{\partial o_j^{(h)}}{\partial h_j} = 1 \quad \frac{\partial h_j}{\partial W_{ij}} = x_i$$

One Hidden Layer : Putting it All Together

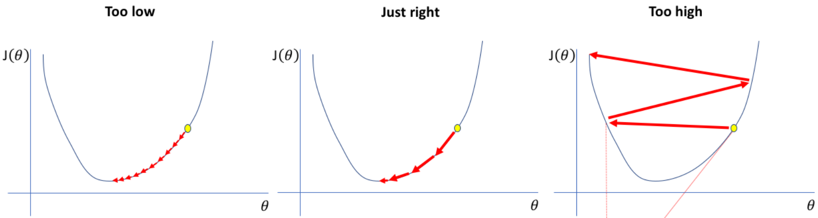
- Last-Layer Weight

$$\frac{\partial \mathscr{L}}{\partial W'_j} = \frac{\partial \mathscr{L}}{\partial o}\frac{\partial o}{\partial z}\frac{\partial z}{\partial W'_j}$$
$$= -(t-o)(o-o^2)h_j$$

- Inner-Layer Weight

$$\frac{\partial \mathscr{L}}{\partial W_{ij}} = \frac{\partial \mathscr{L}}{\partial o}\frac{\partial o}{\partial z}\frac{\partial z}{\partial o_j^{(h)}}\frac{\partial o_j^{(h)}}{\partial h_j}\frac{\partial h_j}{\partial W_{ij}}$$
$$= -(t-o)(o-o^2)W'_j x_i$$

Effect of Learning Rate

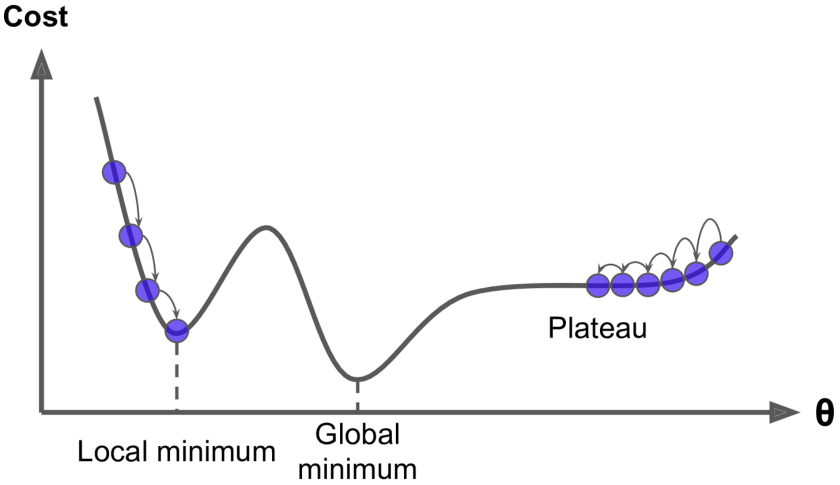


A small learning rate requires many updates before reaching the minimum point

The optimal learning rate swiftly reaches the minimum point

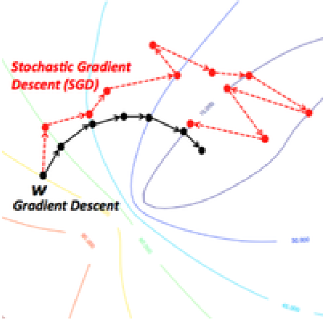
Too large of a learning rate causes drastic updates which lead to divergent behaviors

Local Minima



Stochastic Gradient Descent

- Sample many batches of size b from $X^{d \times n}$.
- $b << n$.
- Allows small incorrect steps during training.
- Better overcomes local minima.



Gradient Descent Modifications

- Momentum
- Nesterov

Momentum

- Original

$$\Delta W = -\eta \frac{\partial \mathcal{L}}{\partial W}$$

- With Momentum

$$M_k = \beta M_{k-1} + \alpha \frac{\partial \mathcal{L}}{\partial W}$$

$$\Delta W = -\eta M_k$$

Nesterov

- Original

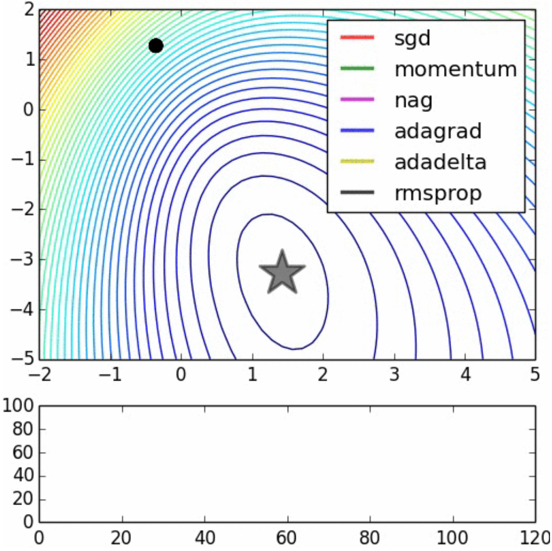
$$\Delta W = -\eta \frac{\partial \mathscr{L}}{\partial W}$$

- With Nesterov

$$N_k = \beta N_{k-1} + \alpha \frac{\partial}{\partial W} \mathscr{L}\left(X, (W - \beta N_{k-1}), t\right)$$

$$\Delta W = -\eta N_k$$

GD Modifications Visualization



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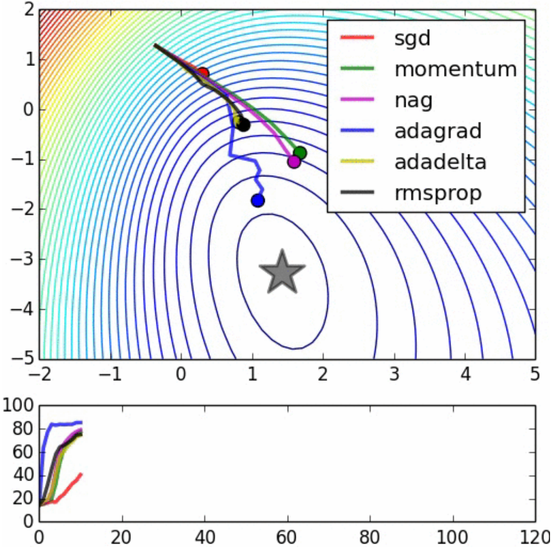

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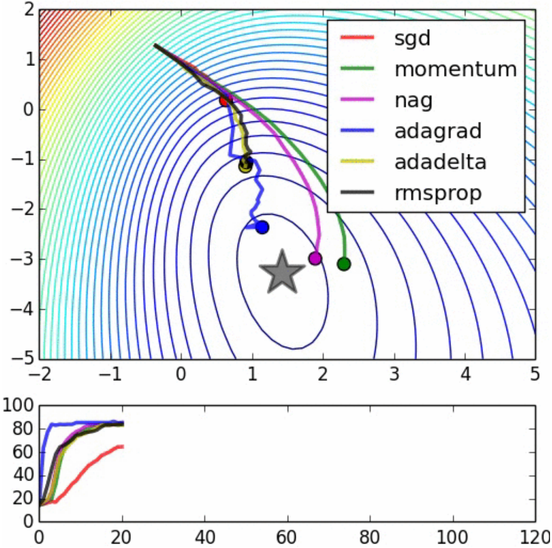

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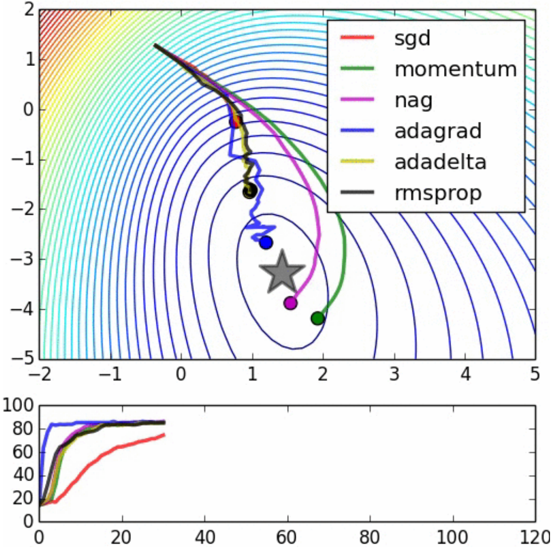

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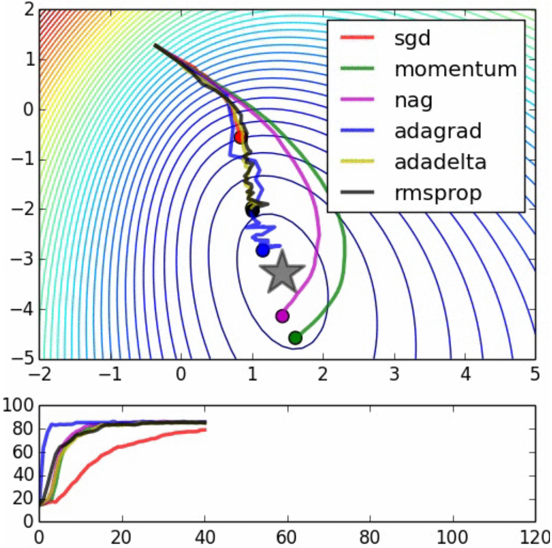

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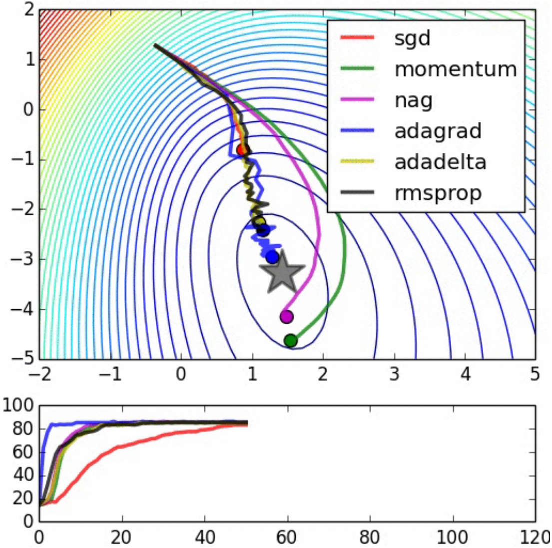

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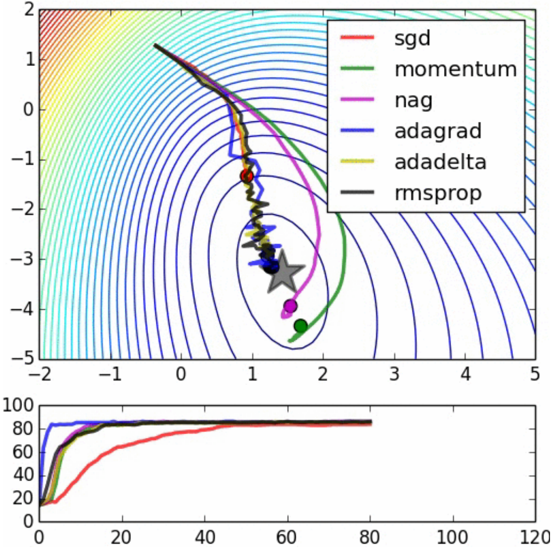

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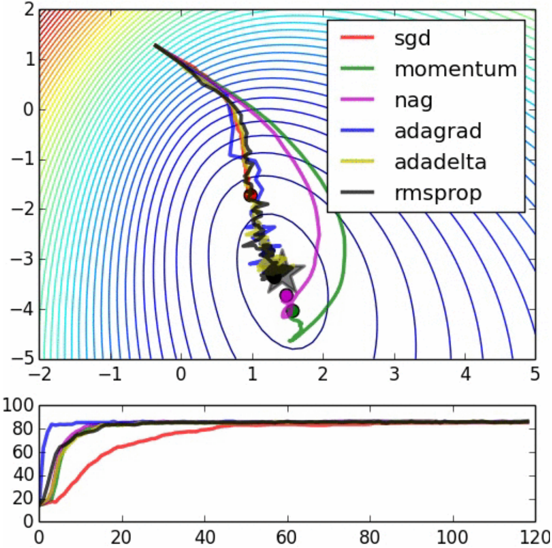
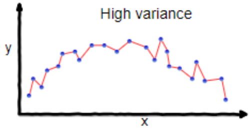
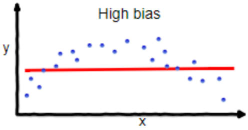


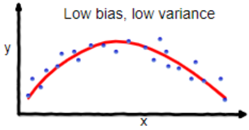
Bias and Variance



overfitting



underfitting



Good balance

Bias and Variance

- In case of bias:
  - Increase model parameters
  - Increase features
  - Lower learning rate
- In case of variance:
  - Increase data
  - Remove features
  - Add regularization terms
  - Raise learning rate