Warm up

Given $x_1, \ldots, x_n \in \mathbb{R}$

Find:

- $\arg\min_z \sum_{i=1}^n (x_i - z)^2$ $= \frac{1}{n} \sum_{i=1}^{n} x_i$
- $\arg\min_z \sum_{i=1}^n |x_i - z|$ $= f(z)$ $=$ median$(x_1, \ldots, x_n)$

$\nabla f(z) = \sum_{i=1}^{n} \nabla |x_i - z| = 0$

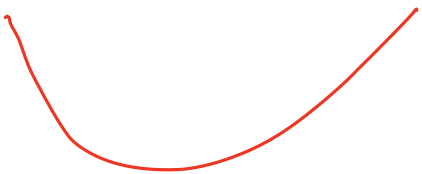
$\frac{\partial}{\partial z} |x_i - z| = \begin{cases} -1 & z < x_i \\ \in [-1,1] & z = x_i \\ 1 & z > x_i \end{cases}$

n=even $\underbrace{\quad\quad\quad}_{n/2}$ $\underbrace{\quad\quad\quad}_{n/2}$ $\nabla f(z) = 0$ $z \in [x_{n/2}, x_{n/2+1}]$ sorted

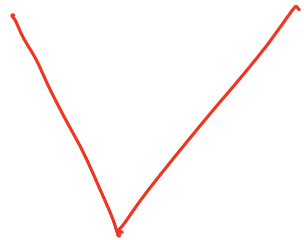
$\cdot\ \cdot\ \cdot\ \cdot\ \cdot\ z\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot$

n=odd $\nabla f(z)$ $z = x_{(n+1)/2}$

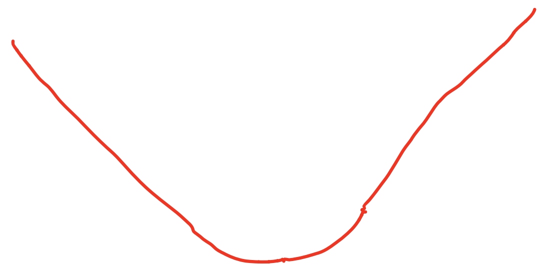
Warm up



$(\cdot)^2$



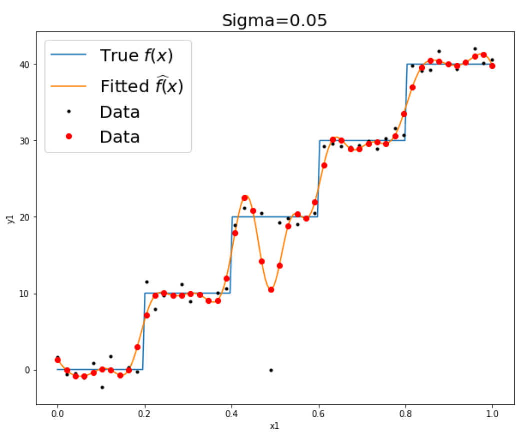
$|\cdot|$

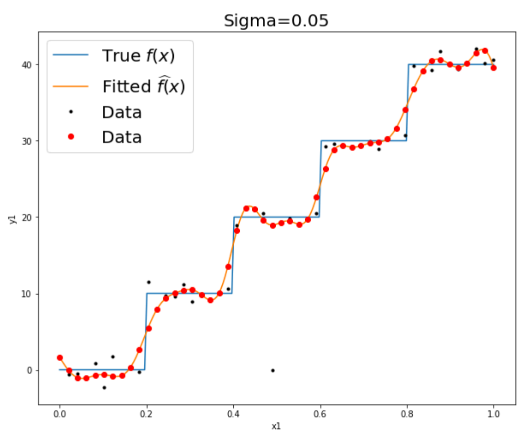


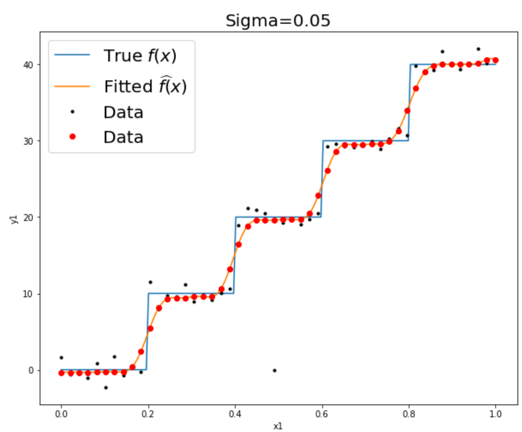
Least squares

Absolute error

Huber







Backprop

Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 27, 2018

©Kevin Jamieson 2018

Backprop

$\Theta^{(1)} \in \mathbb{R}^{5\times 3}$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

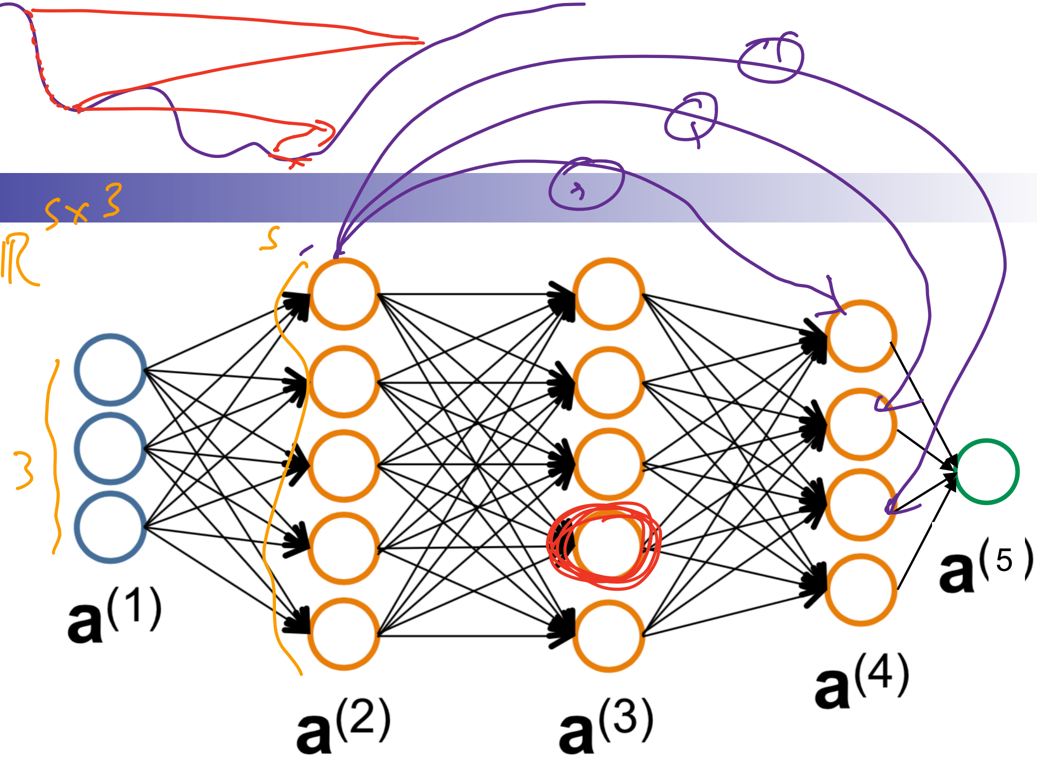
$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$



$$L(y, \hat{y}) = y \log(\hat{y}) + (1 - y)\log(1 - \hat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}}$$

Backprop

$L(y,\hat{y}) = h_L(h_{L-1}(h_{L-2}(\cdots h_1(x))))$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

Gradient Descent

Loop: over examples (x_k, y_k)

For all i,j,l

$$\Theta_{i,j}^{(l)} \leftarrow \Theta_{i,j}^{(l)} - \gamma \frac{\partial L(y,\hat{y})}{\partial \Theta_{i,j}^{(l)}}$$

$$L(y,\hat{y}) = y\log(\hat{y}) + (1-y)\log(1-\hat{y})$$

$$g(z) = \frac{1}{1+e^{-z}}$$

Backprop

$$\frac{\partial L(y,\widehat{y})}{\partial \Theta^{(l)}_{i,j}} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta^{(l)}_{i,j}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = a^{(L+1)}$$

$$z_i^{(l+1)} = \left(\theta^{(l)} a^{(l)}\right)_i$$

$$= \sum_{j=1} \theta_{i,j}^{(l)} a_j^{(l)}$$

$$L(y,\widehat{y}) = y\log(\widehat{y}) + (1-y)\log(1-\widehat{y})$$

$$g(z) = \frac{1}{1+e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$\frac{\partial L(y,\hat{y})}{\partial \Theta^{(l)}_{i,j}} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta^{(l)}_{i,j}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$$g'(z) = g(z)(1-g(z))$$

$$z_k^{(l+1)} = \theta^{(l)} a^{(l)} = \theta^{(l)} g(z^{(l)})$$

$$\delta_i^{(l)} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l)}} = \sum_k \frac{\partial L(y,\hat{y})}{\partial z_k^{(l+1)}} \cdot \frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}}$$

$$= \sum_k \delta_k^{(l+1)} \cdot \Theta^{(l)}_{k,i}\, g'(z_i^{(l)})$$

$$= a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta^{(l)}_{k,i}$$

$$L(y,\hat{y}) = y\log(\hat{y}) + (1-y)\log(1-\hat{y})$$

$$g(z) = \frac{1}{1+e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$\frac{\partial L(y,\widehat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1-a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}$$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = a^{(L+1)}$$

$$L(y,\widehat{y}) = y\log(\widehat{y}) + (1-y)\log(1-\widehat{y})$$

$$g(z) = \frac{1}{1+e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y,\widehat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$\frac{\partial L(y,\hat{y})}{\partial \Theta^{(l)}_{i,j}} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta^{(l)}_{i,j}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}$$

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\hat{y} = a^{(L+1)}$$

$$\begin{aligned}\delta_i^{(L+1)} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(L+1)}} &= \frac{\partial}{\partial z_i^{(L+1)}} \left[y \log(g(z^{(L+1)})) + (1-y)\log(1 - g(z^{(L+1)})) \right] \\ &= \frac{y}{g(z^{(L+1)})} g'(z^{(L+1)}) - \frac{1-y}{1-g(z^{(L+1)})} g'(z^{(L+1)}) \\ &= y - g(z^{(L+1)}) = y - a^{(L+1)}\end{aligned}$$

$$L(y,\hat{y}) = y \log(\hat{y}) + (1-y)\log(1-\hat{y})$$

$$g(z) = \frac{1}{1+e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y,\hat{y})}{\partial z_i^{(l+1)}}$$

Backprop

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = a^{(L+1)}$$

$$\frac{\partial L(y, \widehat{y})}{\partial \Theta_{i,j}^{(l)}} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}} \cdot \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} =: \delta_i^{(l+1)} \cdot a_j^{(l)}$$

$$\delta_i^{(l)} = a_i^{(l)}(1 - a_i^{(l)}) \sum_k \delta_k^{(l+1)} \cdot \Theta_{k,i}$$

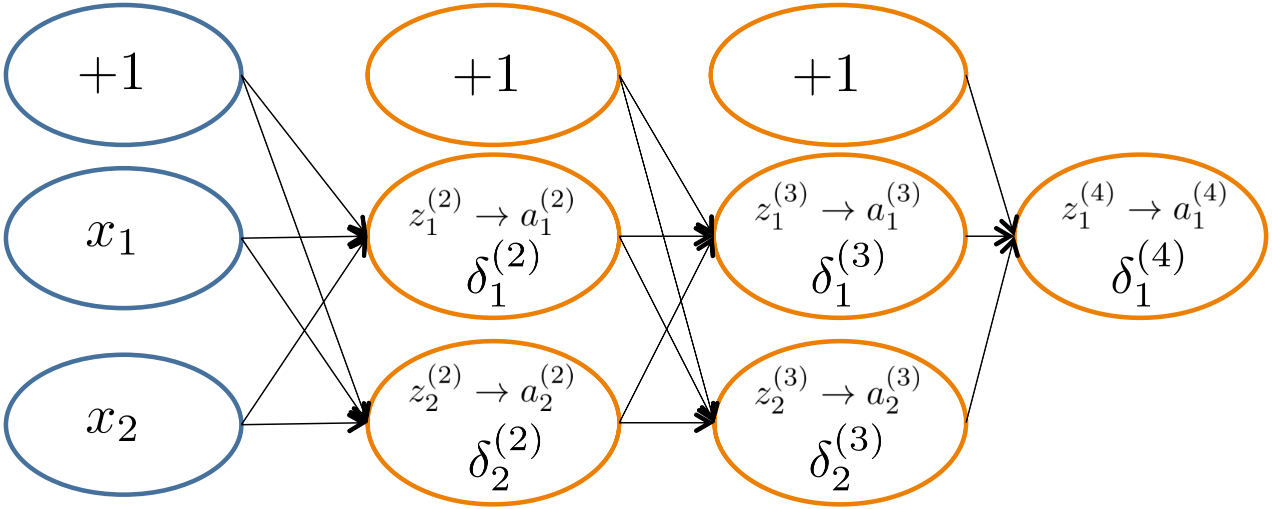
$$\delta^{(L+1)} = y - a^{(L+1)}$$

Recursive Algorithm!

$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1 - y)\log(1 - \widehat{y})$$

$$g(z) = \frac{1}{1 + e^{-z}} \qquad \delta_i^{(l+1)} = \frac{\partial L(y, \widehat{y})}{\partial z_i^{(l+1)}}$$

Backpropagation Intuition

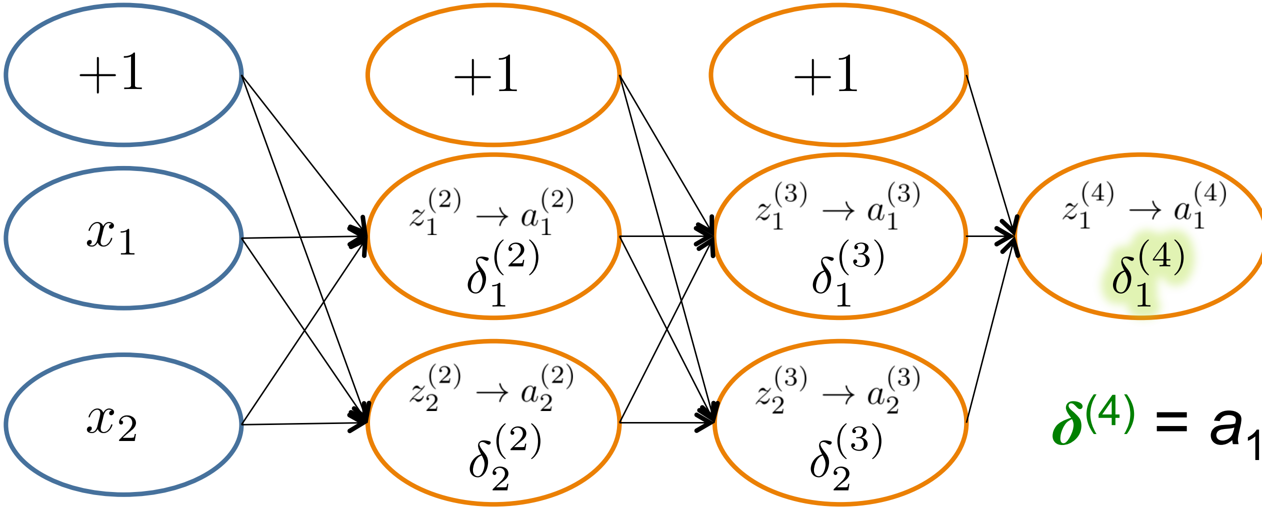


$\delta_j^{(l)}$ = "error" of node *j* in layer *l*

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \mathrm{cost}(\mathbf{x}_i)$

$$\text{where } \mathrm{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

Backpropagation Intuition



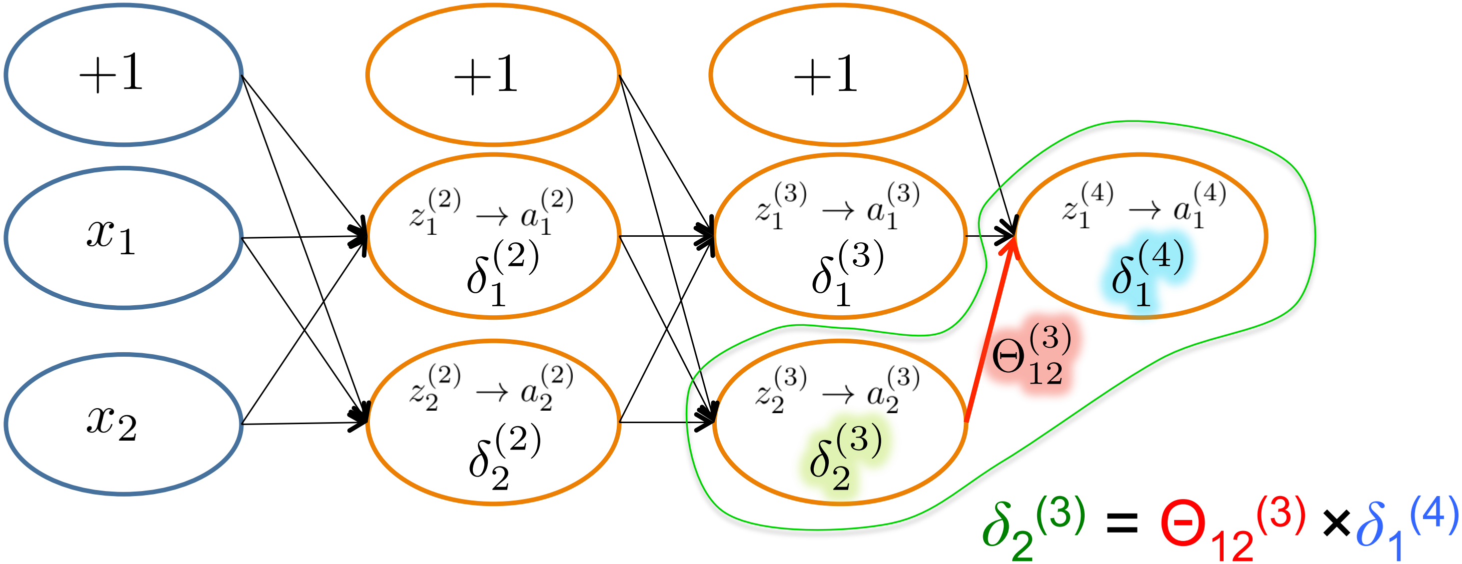
$\boldsymbol{\delta}^{(4)} = a_1^{(4)} - y$

$\delta_j^{(l)}$ = "error" of node *j* in layer *l*

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

$$\text{where } \text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

Backpropagation Intuition

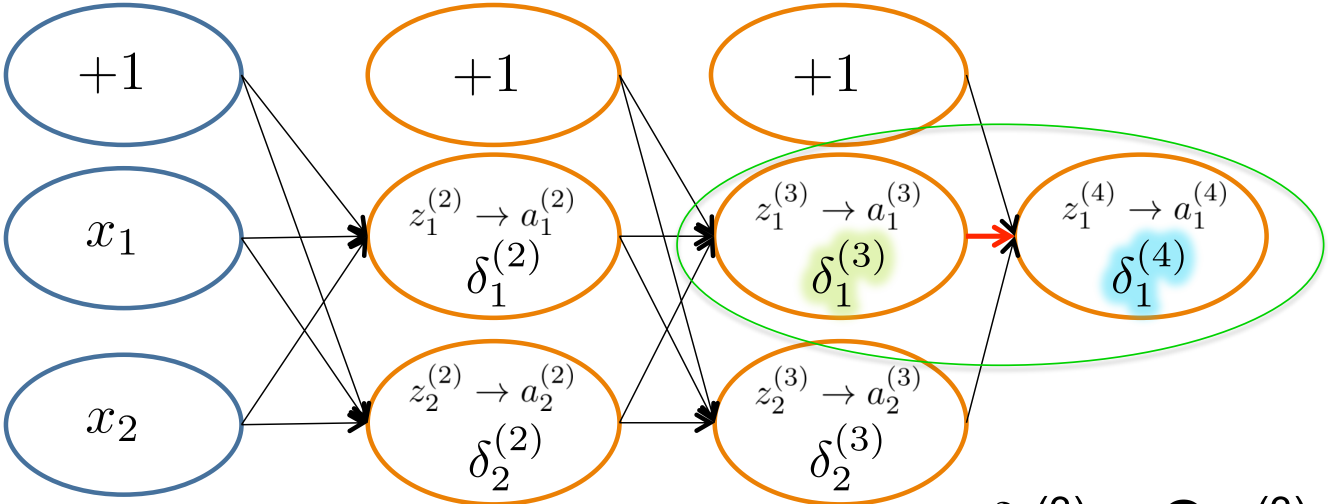


$\delta_j^{(l)}$ = "error" of node *j* in layer *l*

Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

$$\text{where } \text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

Backpropagation Intuition



$\delta_2{}^{(3)} = \Theta_{12}{}^{(3)} \times \delta_1{}^{(4)}$

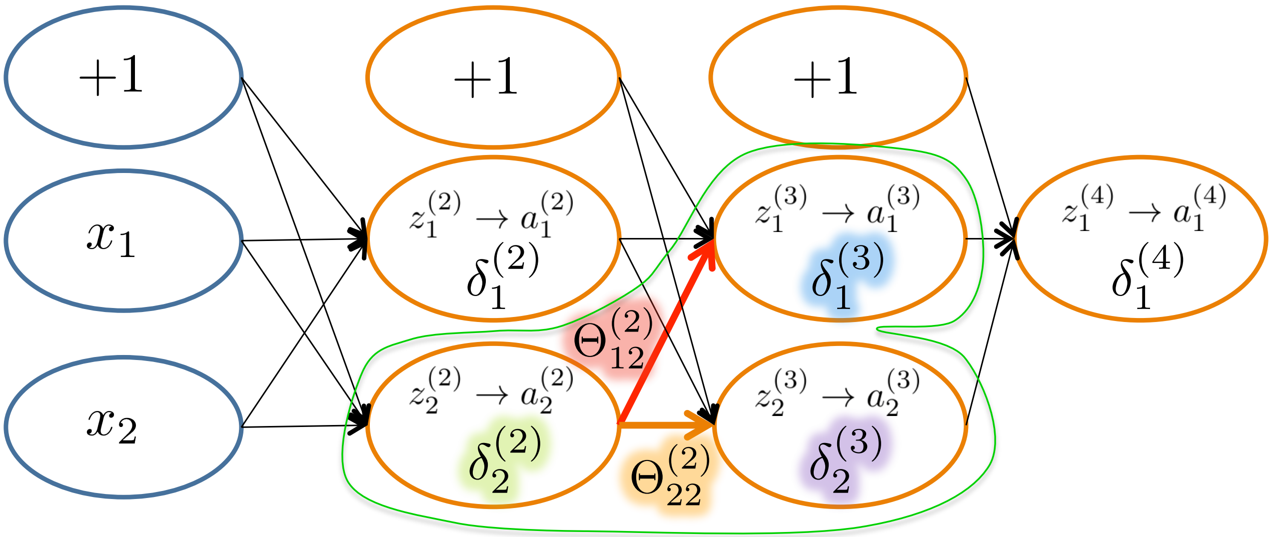
$\delta_1{}^{(3)} = \Theta_{11}{}^{(3)} \times \delta_1{}^{(4)}$

$\delta_j^{(l)}$ = "error" of node *j* in layer *l*

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

$$\text{where } \text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$$

Backpropagation Intuition



$$\delta_2^{(2)} = \Theta_{12}^{(2)} \times \delta_1^{(3)} + \Theta_{22}^{(2)} \times \delta_2^{(3)}$$

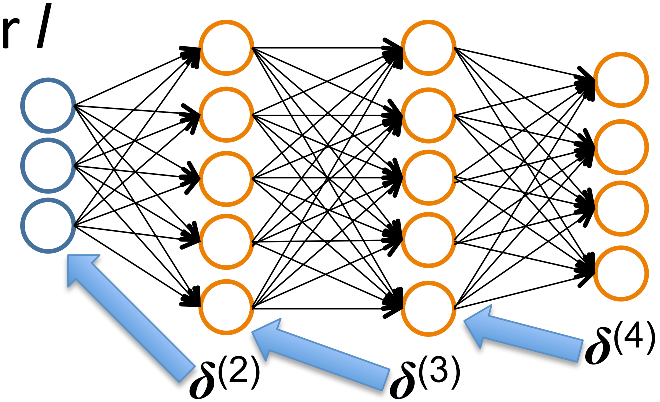
$\delta_j^{(l)}$ = "error" of node *j* in layer *l*

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

$$\text{where } \text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i)\log(1 - h_\Theta(\mathbf{x}_i))$$

Backpropagation: Gradient Computation

Let $\delta_j^{(l)}$ = "error" of node j in layer l



(#layers $L = 4$)

Element-wise product .*

<u>Backpropagation</u>

- $\boldsymbol{\delta}^{(4)} = \mathbf{a}^{(4)} - \mathbf{y}$
- $\boldsymbol{\delta}^{(3)} = (\Theta^{(3)})^{\mathsf{T}}\boldsymbol{\delta}^{(4)} \;.\!*\; g'(\mathbf{z}^{(3)})$
- $\boldsymbol{\delta}^{(2)} = (\Theta^{(2)})^{\mathsf{T}}\boldsymbol{\delta}^{(3)} \;.\!*\; g'(\mathbf{z}^{(2)})$
- (No $\boldsymbol{\delta}^{(1)}$)

$g'(\mathbf{z}^{(3)}) = \mathbf{a}^{(3)} \;.\!*\; (1 - \mathbf{a}^{(3)})$

$g'(\mathbf{z}^{(2)}) = \mathbf{a}^{(2)} \;.\!*\; (1 - \mathbf{a}^{(2)})$

Backpropagation

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)

For each training instance $(\mathbf{x}_i, y_i)$:

Set $\mathbf{a}^{(1)} = \mathbf{x}_i$

Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation

Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_i$

Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \ldots, \boldsymbol{\delta}^{(2)}\}$

Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

D$^{(l)}$ is the matrix of partial derivatives of $J(\Theta)$

Training a Neural Network via Gradient Descent with Backprop

Given: training set $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
Initialize all $\Theta^{(l)}$ randomly (NOT to 0!)
Loop // each iteration is called an epoch

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient)
For each training instance $(\mathbf{x}_i, y_i)$:
Set $\mathbf{a}^{(1)} = \mathbf{x}_i$
Compute $\{\mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(L)}\}$ via forward propagation
Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y_i$
Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \ldots, \boldsymbol{\delta}^{(2)}\}$
Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute avg regularized gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & \text{if } j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & \text{otherwise} \end{cases}$

Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$
Until weights converge or max #epochs is reached

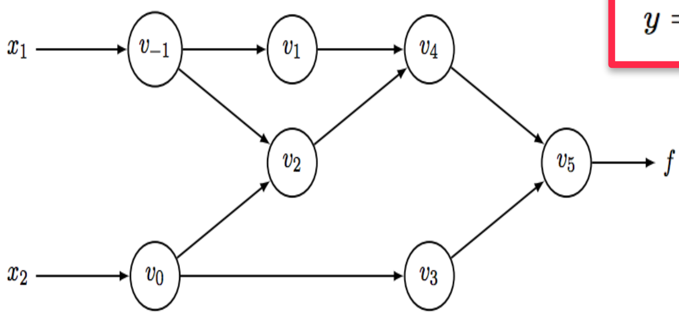
Backpropagation

Based on slide by Andrew Ng

Autodiff

Backprop for this simple network architecture is a special case of ***reverse-mode auto-differentiation***:

$$\boxed{y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)}$$



Forward Primal Trace		
v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

Reverse Adjoint (Derivative) Trace			
$\bar{\boldsymbol{x}}_1$	$= \bar{\boldsymbol{v}}_{-1}$		$= \mathbf{5.5}$
$\bar{\boldsymbol{x}}_2$	$= \bar{\boldsymbol{v}}_0$		$= \mathbf{1.716}$
$\bar{v}_{-1}$	$= \bar{v}_{-1} + \bar{v}_1 \frac{\partial v_1}{\partial v_{-1}}$	$= \bar{v}_{-1} + \bar{v}_1 / v_{-1}$	$= 5.5$
$\bar{v}_0$	$= \bar{v}_0 + \bar{v}_2 \frac{\partial v_2}{\partial v_0}$	$= \bar{v}_0 + \bar{v}_2 \times v_{-1}$	$= 1.716$
$\bar{v}_{-1}$	$= \bar{v}_2 \frac{\partial v_2}{\partial v_{-1}}$	$= \bar{v}_2 \times v_0$	$= 5$
$\bar{v}_0$	$= \bar{v}_3 \frac{\partial v_3}{\partial v_0}$	$= \bar{v}_3 \times \cos v_0$	$= -0.284$
$\bar{v}_2$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_2}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_1$	$= \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	$= \bar{v}_4 \times 1$	$= 1$
$\bar{v}_3$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_3}$	$= \bar{v}_5 \times (-1)$	$= -1$
$\bar{v}_4$	$= \bar{v}_5 \frac{\partial v_5}{\partial v_4}$	$= \bar{v}_5 \times 1$	$= 1$
$\bar{v}_5$	$= \bar{y}$	$= 1$	

This is the special sauce in Tensorflow, PyTorch, Theano, …

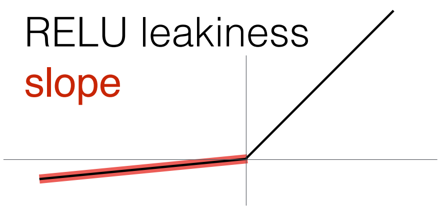
Real networks

Residual Network of [HeZhangRenSun'15]

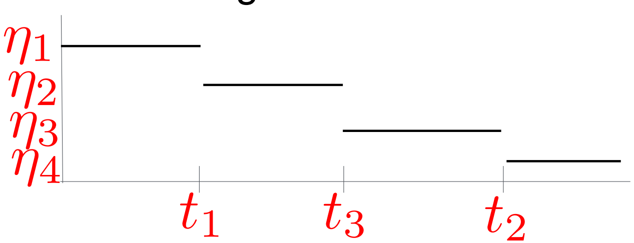
Modern networks have dozens of parameters to tune.

Data augmentation?
Batch norm?

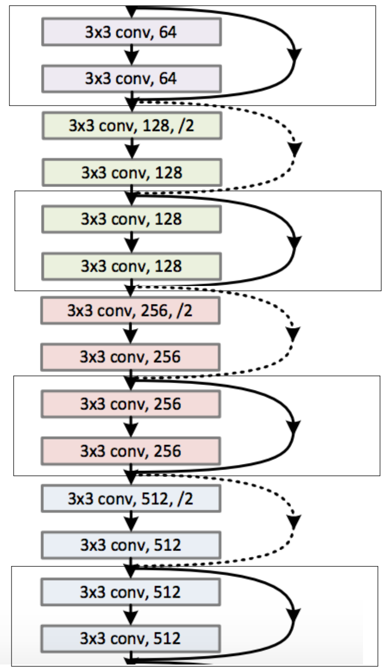
RELU leakiness
slope



Learning rate schedule



batchsize



Reduce spatial dimension

Reduce spatial dimension

Reduce spatial dimension

n0 layers of f0 filters

n1 layers of f1 filters

n2 layers of f2 filters

n3 layers of f3 filters

Trees

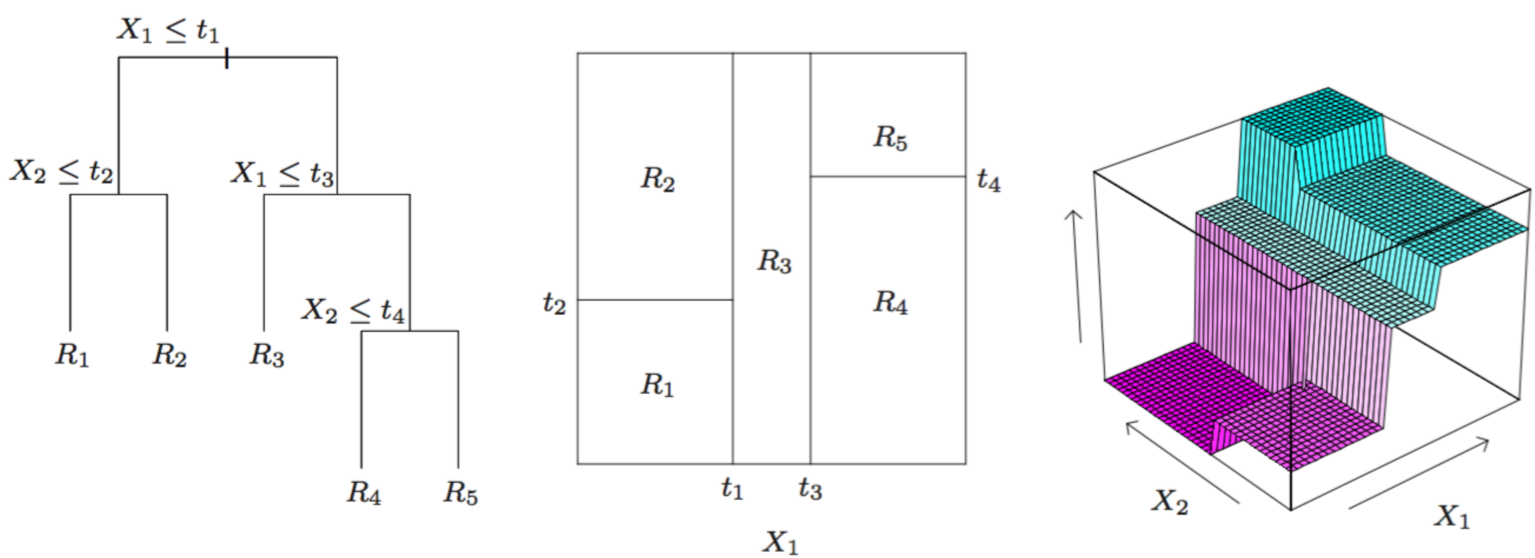
Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 29, 2018

Trees

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

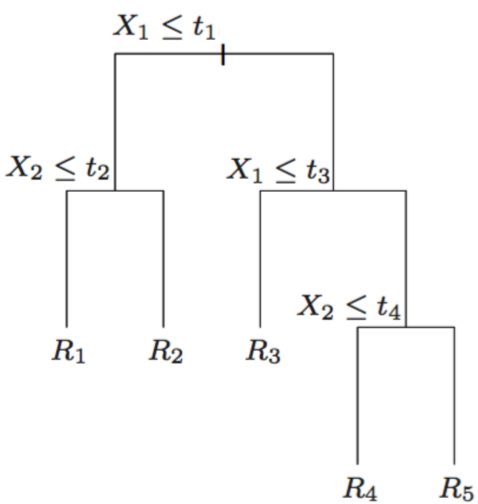
Build a binary tree, splitting along axes



Trees

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

Build a binary tree, splitting along axes

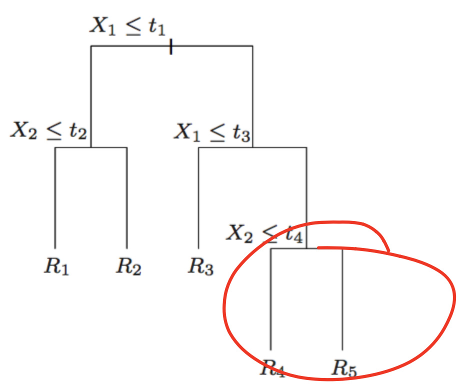


How do you split?

When do you stop?

Learning decision trees

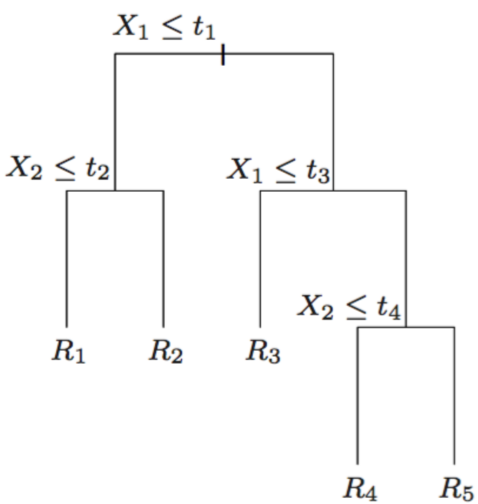
- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute
  - Split on $\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$
- Recurse
- Prune



$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

Trees

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$



- Trees
  - **have low bias, high variance**
  - deal with categorial variables well
  - intuitive, interpretable
  - good software exists
  - Some theoretical guarantees

Random Forests

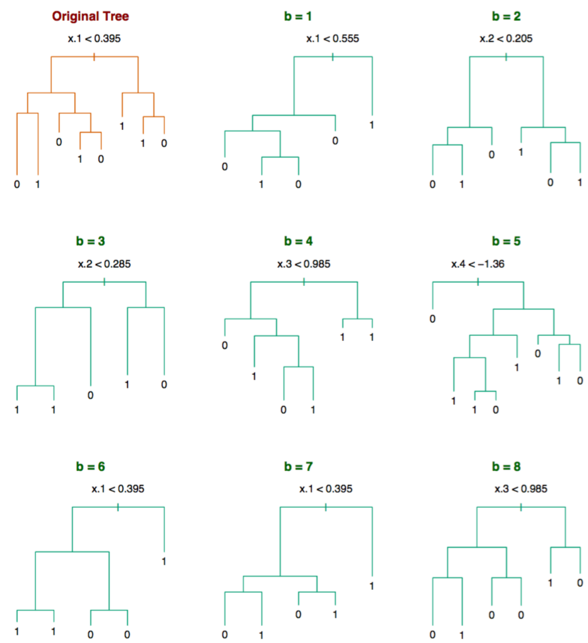
Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 29, 2018

Random Forests

Tree methods have **low bias** but **high variance.**

One way to reduce variance is to construct a lot of “lightly correlated” trees and average them:



“Bagging:” Bootstrap aggregating

Random Forrests

Algorithm 15.1 *Random Forest for Regression or Classification.*

1. For $b = 1$ to B:
   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.
   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.
      i. Select m variables at random from the p variables.
      ii. Pick the best variable/split-point among the m.
      iii. Split the node into two daughter nodes.
2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression: $\hat{f}_{\rm rf}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.   m~p/3

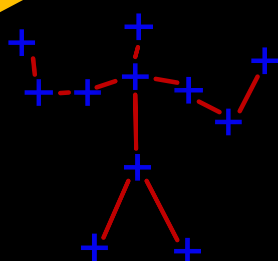
Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\rm rf}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.   m~sqrt(p)

The Kinect pose estimation pipeline

capture
depth image &
remove bg

infer
body parts
per pixel

cluster pixels to
hypothesize
body joint
positions

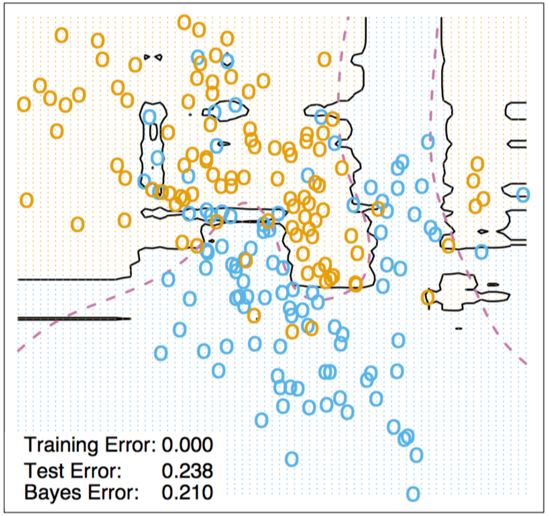


fit model &
track skeleton

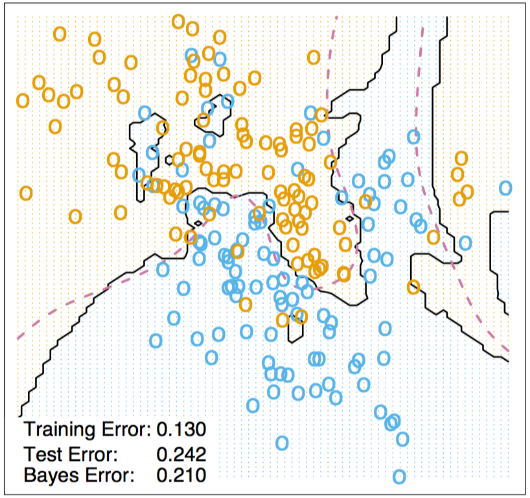
https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/CVPR20201120-20Final20Video.mp4

Random Forests

Random forrest



3 nearest neighbor



Random Forests

Given random variables $Y_1, Y_2, \ldots, Y_B$ with
$\mathbb{E}[Y_i] = y$, $\mathbb{E}[(Y_i - y)^2] = \sigma^2$, $\mathbb{E}[(Y_i - y)(Y_j - y)] = \rho\sigma^2$

The Yi's are identically distributed but **not** independent

$$\mathbb{E}[(\frac{1}{B}\sum_{i=1}^{B} Y_i - y)^2] = \frac{1}{B^2}\left(\sum_i \mathbb{E}[(Y_i - y)^2] + \sum_{i \neq j} \mathbb{E}[(Y_i - y)(Y_j - y)]\right)$$

$$= \frac{1}{B^2}\left(B\sigma^2 + B(B-1)\rho\sigma^2\right)$$

$$= \frac{1}{B}\sigma^2 + \left(1 - \frac{1}{B}\right)\rho\sigma^2$$

Random Forests

- Random Forests
  - **have low bias, low variance**
  - deal with categorial variables well
  - not that intuitive or interpretable
  - Notion of confidence estimates
  - good software exists
  - Some theoretical guarantees
  - **works well with default hyperparameters**

Boosting

Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 29, 2018

Boosting

- 1988 Kearns and Valiant: "Can **weak learners** be combined to create a **strong learner?**"

Weak learner definition (informal):

An algorithm $\mathcal{A}$ is a *weak learner* for a hypothesis class $\mathcal{H}$ that maps $\mathcal{X}$ to $\{-1,1\}$ if for all input distributions over $\mathcal{X}$ and $h \in \mathcal{H}$, we have that $\mathcal{A}$ correctly classifies h with error at most $1/2 - \gamma$

Boosting

- 1988 Kearns and Valiant: “Can **weak learners** be combined to create a **strong learner?**”

Weak learner definition (informal):

An algorithm $\mathcal{A}$ is a *weak learner* for a hypothesis class $\mathcal{H}$ that maps $\mathcal{X}$ to $\{-1, 1\}$ if for all input distributions over $\mathcal{X}$ and $h \in \mathcal{H}$, we have that $\mathcal{A}$ correctly classifies h with error at most $1/2 - \gamma$

- 1990 Robert Schapire: “Yup!”
- 1995 Schapire and Freund: “Practical for 0/1 loss” AdaBoost

Boosting

- 1988 Kearns and Valiant: "Can **weak learners** be combined to create a **strong learner?**"

Weak learner definition (informal):

An algorithm $\mathcal{A}$ is a *weak learner* for a hypothesis class $\mathcal{H}$ that maps $\mathcal{X}$ to $\{-1, 1\}$ if for all input distributions over $\mathcal{X}$ and $h \in \mathcal{H}$, we have that $\mathcal{A}$ correctly classifies h with error at most $1/2 - \gamma$

- 1990 Robert Schapire: "Yup!"
- 1995 Schapire and Freund: "Practical for 0/1 loss" AdaBoost
- 2001 Friedman: "Practical for arbitrary losses"

Boosting

- 1988 Kearns and Valiant: “Can **weak learners** be combined to create a **strong learner?**”

Weak learner definition (informal):

An algorithm $\mathcal{A}$ is a *weak learner* for a hypothesis class $\mathcal{H}$ that maps $\mathcal{X}$ to $\{-1, 1\}$ if for all input distributions over $\mathcal{X}$ and $h \in \mathcal{H}$, we have that $\mathcal{A}$ correctly classifies h with error at most $1/2 - \gamma$

- 1990 Robert Schapire: “Yup!”
- 1995 Schapire and Freund: “Practical for 0/1 loss” AdaBoost
- 2001 Friedman: “Practical for arbitrary losses”
- 2014 Tianqi Chen: “Scale it up!” XGBoost

Boosting and Additive Models

Machine Learning – CSE546
Kevin Jamieson
University of Washington

November 29, 2018

Additive models

- Consider the first algorithm we used to get good classification for MNIST. Given: $\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$
- Generate **random** functions: $\phi_t : \mathbb{R}^d \to \mathbb{R} \quad t = 1, \dots, p$
- Learn some weights: $$\widehat{w} = \arg\min_w \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i) \right)$$
- Classify new data: $$f(x) = \text{sign}\left(\sum_{t=1}^p \widehat{w}_t \phi_t(x) \right)$$

Additive models

- Consider the first algorithm we used to get good classification for MNIST. Given: $\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$
- Generate **random** functions: $\phi_t : \mathbb{R}^d \to \mathbb{R} \quad t = 1, \dots, p$
- Learn some weights: $$\widehat{w} = \arg\min_w \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i)\right)$$
- Classify new data: $$f(x) = \text{sign}\left(\sum_{t=1}^p \widehat{w}_t \phi_t(x)\right)$$

An interpretation:
Each $\phi_t(x)$ is a classification rule that we are assigning some weight $\widehat{w}_t$

Additive models

- Consider the first algorithm we used to get good classification for MNIST. Given: $\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$
- Generate **random** functions: $\phi_t : \mathbb{R}^d \to \mathbb{R} \quad t = 1, \dots, p$
- Learn some weights: $$\widehat{w} = \arg\min_w \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i)\right)$$
- Classify new data: $$f(x) = \text{sign}\left(\sum_{t=1}^p \widehat{w}_t \phi_t(x)\right)$$

An interpretation:
Each $\phi_t(x)$ is a classification rule that we are assigning some weight $\widehat{w}_t$

$$\widehat{w}, \widehat{\phi}_1, \dots, \widehat{\phi}_t = \arg \min_{w, \phi_1, \dots, \phi_p} \sum_{i=1}^n \text{Loss}\left(y_i, \sum_{t=1}^p w_t \phi_t(x_i)\right)$$

is in general computationally hard

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ

Examples: $b(x, \gamma) = \dfrac{1}{1 + e^{-\gamma^T x}}$

$b(x, \gamma) = \gamma_1 \mathbf{1}\{x_3 \leq \gamma_2\}$

Algorithm 10.2 *Forward Stagewise Additive Modeling.*

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:

   (a) Compute

   $$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$

   (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.

Idea: greedily add one function at a time

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ

Examples: $b(x, \gamma) = \dfrac{1}{1 + e^{-\gamma^T x}}$

$b(x, \gamma) = \gamma_1 \mathbf{1}\{x_3 \leq \gamma_2\}$

Algorithm 10.2 *Forward Stagewise Additive Modeling.*

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
   (a) Compute
   $$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$
   (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.

Idea: greedily add one function at a time

AdaBoost: $b(x, \gamma)$: classifiers to $\{-1, 1\}$

$$L(y, f(x)) = \exp(-y f(x))$$

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ

Examples: $b(x, \gamma) = \dfrac{1}{1 + e^{-\gamma^T x}}$

$b(x, \gamma) = \gamma_1 \mathbf{1}\{x_3 \leq \gamma_2\}$

Algorithm 10.2 *Forward Stagewise Additive Modeling.*

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
   (a) Compute
   $$(\beta_m, \gamma_m) = \arg\min_{\beta, \gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$
   (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.

Idea: greedily add one function at a time

Boosted Regression Trees: $L(y, f(x)) = (y - f(x))^2$

$b(x, \gamma)$: regression trees

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ

Examples: $b(x, \gamma) = \dfrac{1}{1 + e^{-\gamma^T x}}$

$b(x, \gamma) = \gamma_1 \mathbf{1}\{x_3 \leq \gamma_2\}$

Algorithm 10.2 *Forward Stagewise Additive Modeling.*

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
   (a) Compute
   $$(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).$$
   (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.

Idea: greedily add one function at a time

Boosted Regression Trees: $L(y, f(x)) = (y - f(x))^2$

$$\begin{aligned} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)) &= (y_i - f_{m-1}(x_i) - \beta b(x_i; \gamma))^2 \\ &= (r_{im} - \beta b(x_i; \gamma))^2, \qquad r_{im} = y_i - f_{m-1}(x_i) \end{aligned}$$

Efficient: No harder than learning regression trees!

Forward Stagewise Additive models

$b(x, \gamma)$ is a function with parameters γ

Examples: $b(x, \gamma) = \dfrac{1}{1 + e^{-\gamma^T x}}$

$b(x, \gamma) = \gamma_1 \mathbf{1}\{x_3 \leq \gamma_2\}$

Algorithm 10.2 *Forward Stagewise Additive Modeling.*

1. Initialize $f_0(x) = 0$.
2. For $m = 1$ to M:
   (a) Compute
   $$\boxed{(\beta_m, \gamma_m) = \arg\min_{\beta, \gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)).}$$
   (b) Set $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$.

Idea: greedily add one function at a time

Boosted Logistic Trees: $L(y, f(x)) = y \log(f(x)) + (1 - y) \log(1 - f(x))$

$b(x, \gamma)$: regression trees

Computationally hard to update

Gradient Boosting

Least squares, exponential loss easy. But what about cross entropy? Huber?

Algorithm 10.3 *Gradient Tree Boosting Algorithm.*

1. Initialize $f_0(x) = \arg\min_\gamma \sum_{i=1}^N L(y_i, \gamma)$.
2. For $m = 1$ to M:

   (a) For $i = 1, 2, \ldots, N$ compute

   $$r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}.$$

   (b) Fit a regression tree to the targets r_{im} giving terminal regions $R_{jm},\ j = 1, 2, \ldots, J_m$.

   (c) For $j = 1, 2, \ldots, J_m$ compute

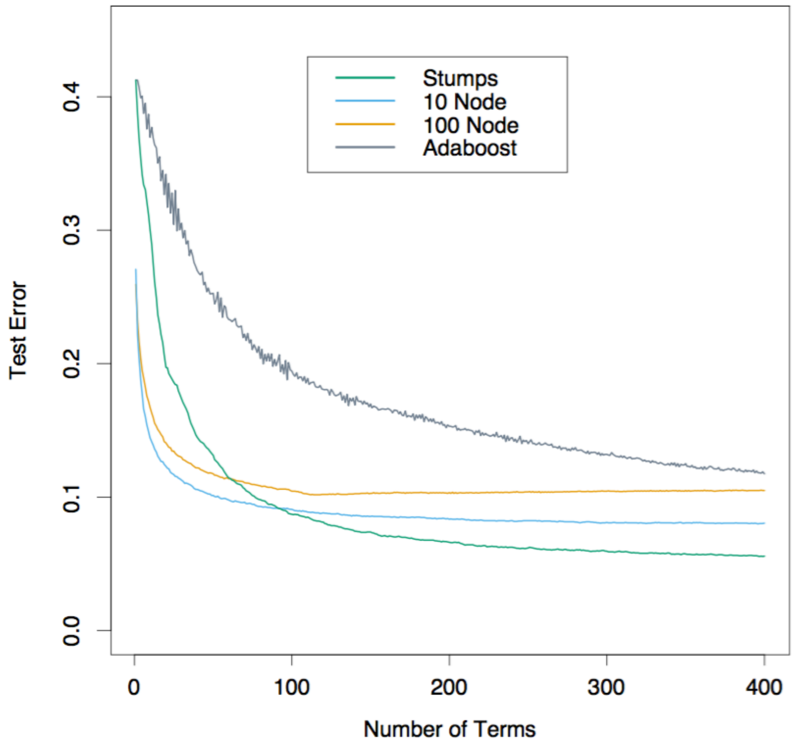
   $$\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma\right).$$

   (d) Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.
3. Output $\hat{f}(x) = f_M(x)$.

LS fit regression tree to n-dimensional gradient, take a step in that direction

Gradient Boosting

Least squares, 0/1 loss easy. But what about cross entropy? Huber?



AdaBoost uses 0/1 loss,
all other trees are minimizing
binomial deviance

Additive models

- Boosting is popular at parties: Invented by theorists, heavily adopted by practitioners.

Additive models

- Boosting is popular at parties: Invented by theorists, heavily adopted by practitioners.
- Computationally efficient with “weak” learners. But can also use trees! Boosting can scale.
- Kind of like sparsity?

Additive models

- Boosting is popular at parties: Invented by theorists, heavily adopted by practitioners.
- Computationally efficient with “weak” learners. But can also use trees! Boosting can scale.
- Kind of like sparsity?
- Gradient boosting generalization with good software packages (e.g., *XGBoost)*. Effective on Kaggle
- Robust to overfitting and can be dealt with with “shrinkage” and “sampling”

Bagging versus Boosting

- Bagging *averages* many **low-bias**, **lightly dependent** classifiers to reduce the variance
- Boosting *learns* linear combination of **high-bias**, **highly dependent** classifiers to reduce error
- Empirically, boosting appears to outperform bagging