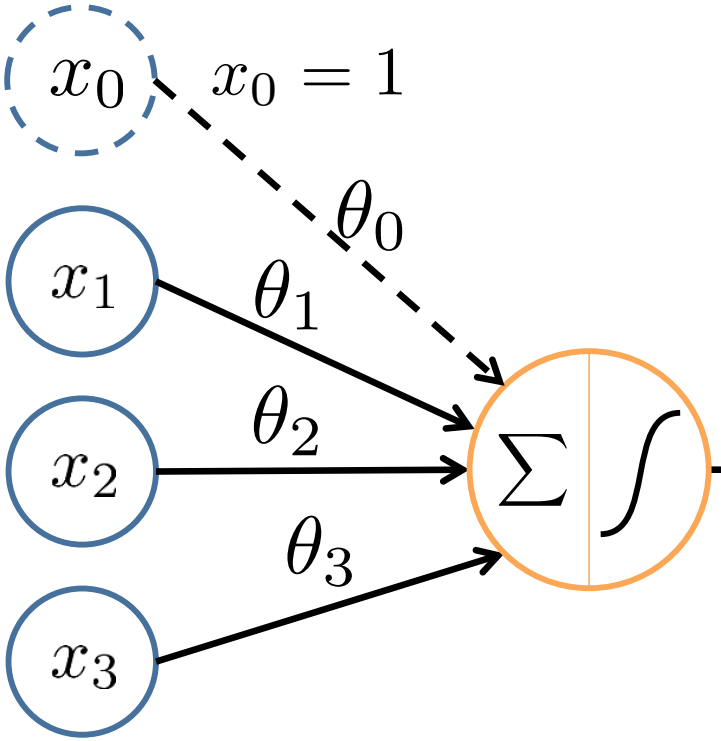
Neural Networks

Matt Golub
Hunter Schafer

UNIVERSITY of WASHINGTON

Single Node



$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

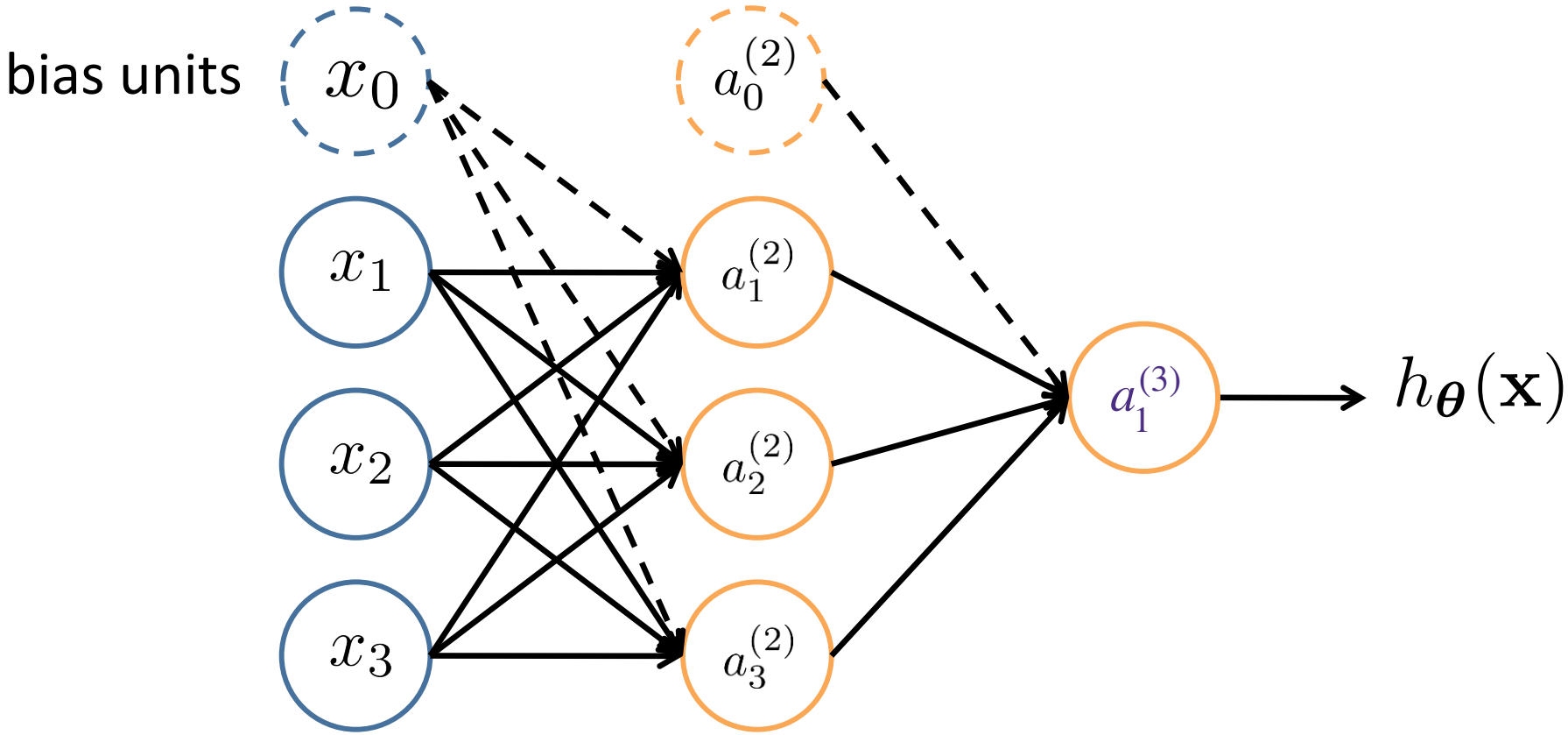
$a_1^{(3)}$

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \sigma(\boldsymbol{\theta}^\top \mathbf{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \mathbf{x}}}$$

Binary Logistic Regression

Sigmoid (logistic) activation function: $g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}$

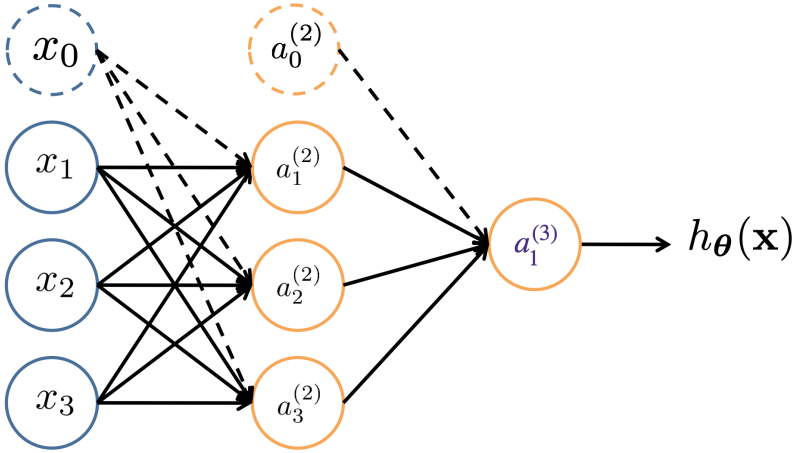
Neural Network



Layer 1 (Input Layer)

Layer 2 (Hidden Layer)

Layer 3 (Output Layer)



$a_i^{(j)}$ = "activation" of unit *i* in layer *j*

$\Theta^{(j)}$ = weight matrix stores parameters from layer *j* to layer *j* + 1

$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

If network has s_j units in layer *j* *and* s_{j+1} units in layer *j*+1, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j+1)$.

$$\Theta^{(1)} \in \mathbb{R}^{3\times 4} \qquad \Theta^{(2)} \in \mathbb{R}^{1\times 4}$$

Multi-layer Neural Network - Binary Classification

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

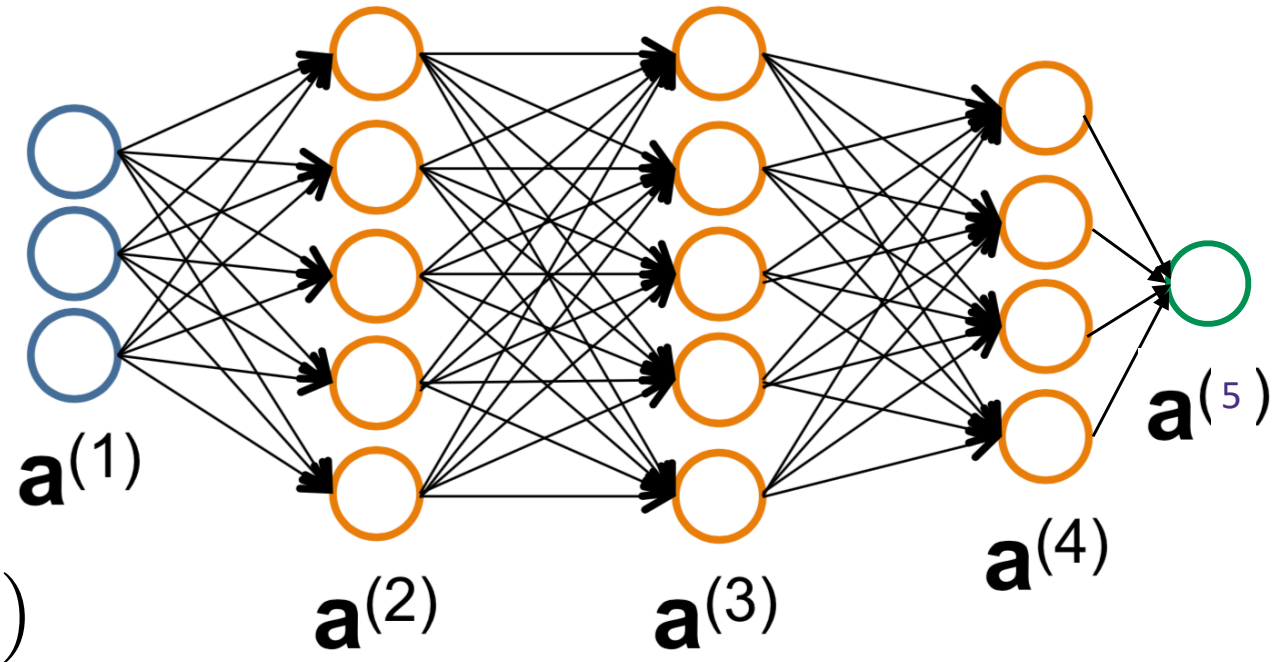
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

$$\hat{y} = g(\Theta^{(L)} a^{(L)})$$



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

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

Binary Logistic Regression

Multi-layer Neural Network - Binary Classification

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

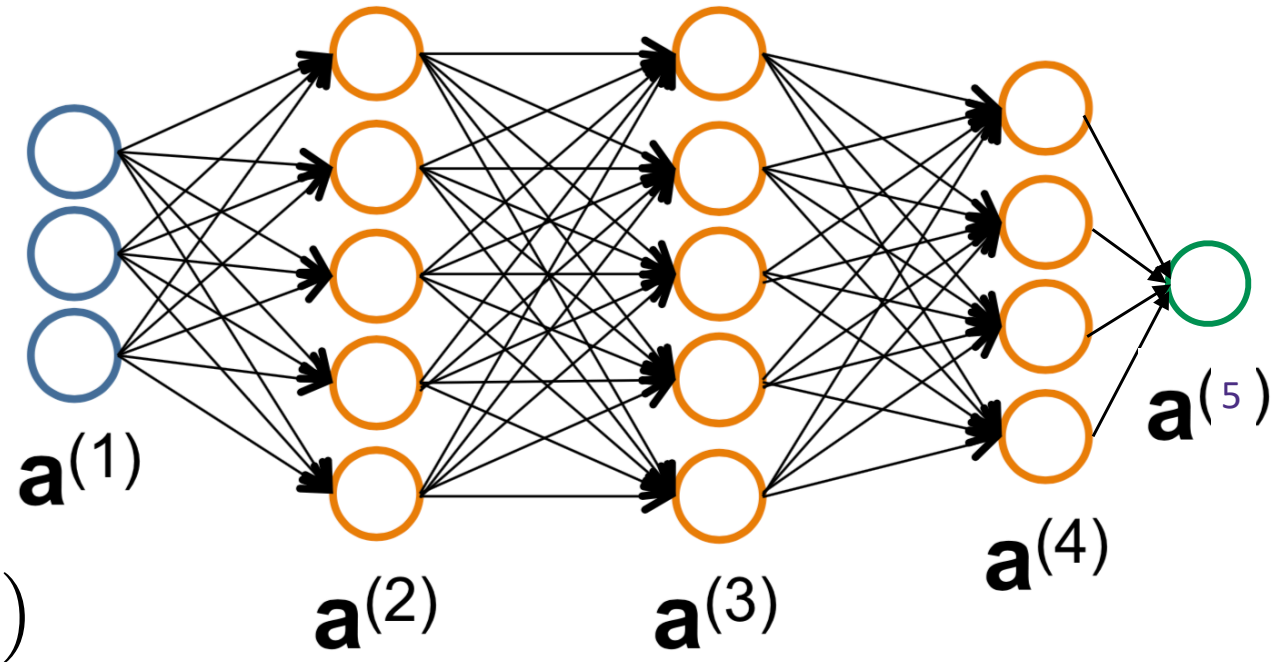
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

$$\hat{y} = \sigma(\Theta^{(L)} a^{(L)})$$



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

$$g(z) = \max\{0, z\} \quad \sigma(z) = \frac{1}{1 + e^{-z}}$$

Binary Logistic Regression

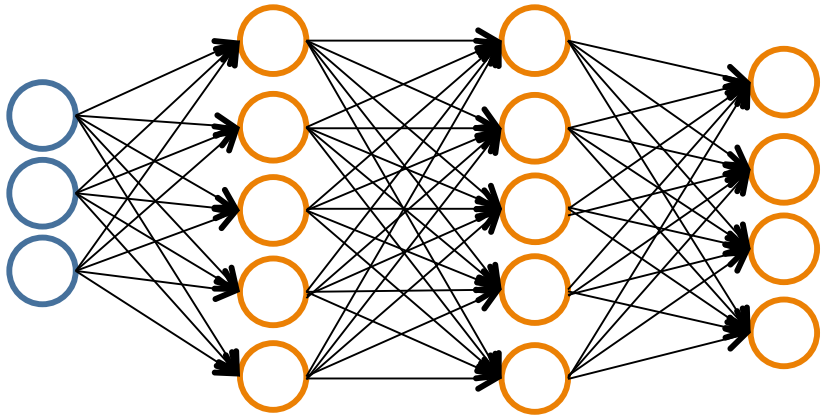
Multiple Output Units: One-vs-Rest

Pedestrian

Car

Motorcycle

Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

Multi-class Logistic Regression

We want:

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

when motorcycle

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

when truck

Multi-layer Neural Network - Regression

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

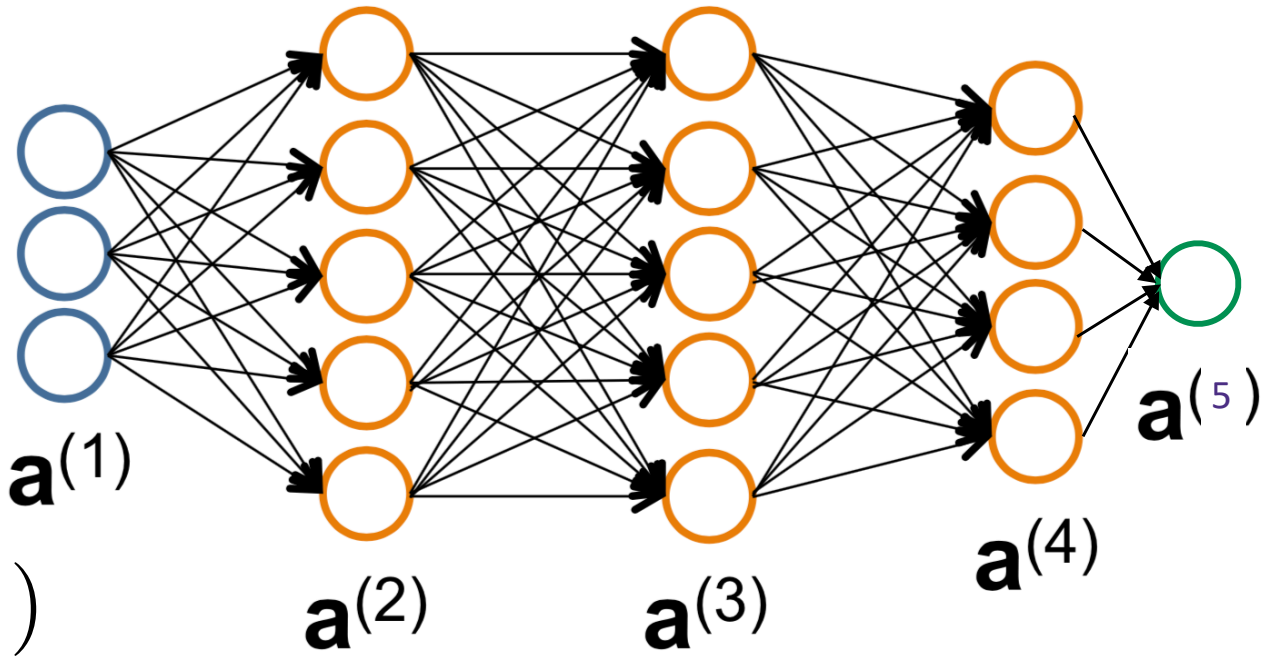
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

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

$$\vdots$$

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



$$L(y, \hat{y}) = (y - \hat{y})^2$$

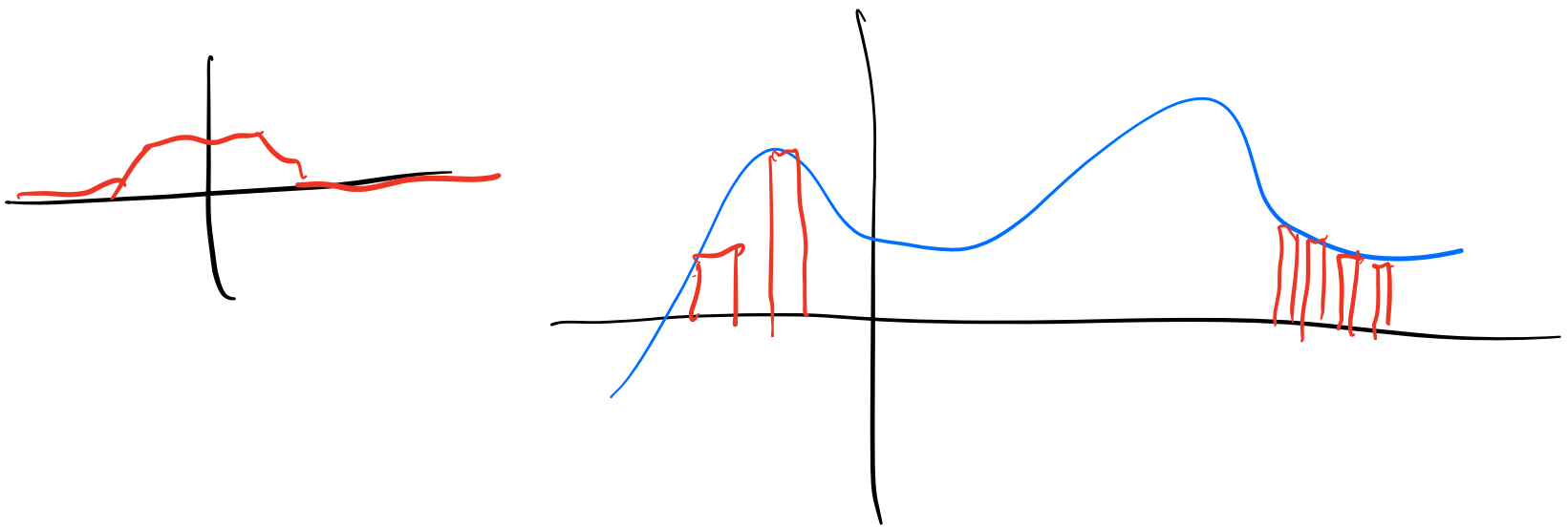
$$g(z) = \max\{0, z\}$$

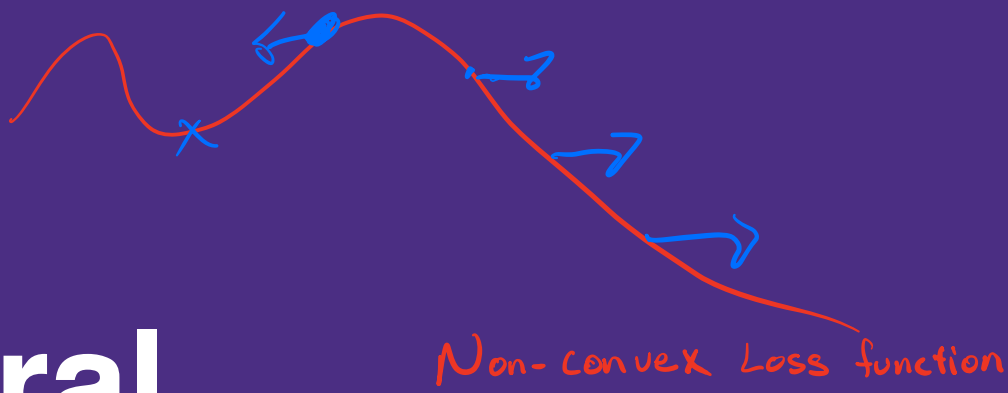
Regression

Neural Networks are arbitrary function approximators

Theorem 10 (Two-Layer Networks are Universal Function Approximators). *Let F be a continuous function on a bounded subset of D-dimensional space. Then there exists a two-layer neural network $\hat{F}$ with a finite number of hidden units that approximate F arbitrarily well. Namely, for all $\boldsymbol{x}$ in the domain of F, $\left|F(\boldsymbol{x}) - \hat{F}(\boldsymbol{x})\right| < \epsilon$.*

Cybenko, Hornik (theorem reproduced from CIML, Ch. 10)





Training Neural Networks

Matt Golub
Hunter Schafer

UNIVERSITY of WASHINGTON

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

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

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

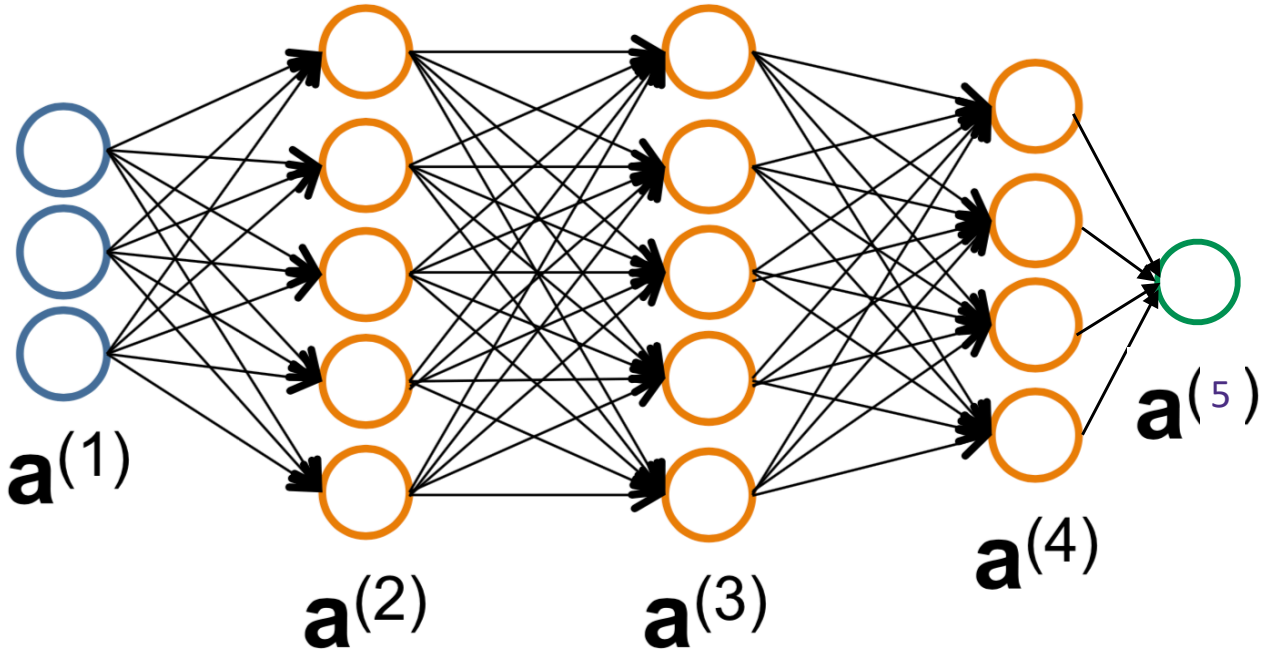
$$\vdots$$

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

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

$$\vdots$$

$$\hat{y} = g(\Theta^{(L)} a^{(L)})$$



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

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

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \hat{y}) \qquad \forall l$

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \widehat{y}) \qquad \forall l$

Seems simple enough, why are packages like PyTorch, Tensorflow, Theano, Cafe, MxNet synonymous with deep learning?

1. Automatic differentiation

Gradient Descent: $$\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \widehat{y}) \qquad \forall l$$

Seems simple enough, why are packages like PyTorch, Tensorflow, Theano, Cafe, MxNet synonymous with deep learning?

1. Automatic differentiation

2. Convenient libraries

Gradient Descent:

Seems simple enough,
Theano, Cafe, MxNet s

1. Automatic differ

2. Convenient libra

```python
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        # 1 input image channel, 6 output channels, 3x3 square convolution
        # kernel
        self.conv1 = nn.Conv2d(1, 6, 3)
        self.conv2 = nn.Conv2d(6, 16, 3)
        # an affine operation: y = Wx + b
        self.fc1 = nn.Linear(16 * 6 * 6, 120)  # 6*6 from image dimension
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)

    def forward(self, x):
        # Max pooling over a (2, 2) window
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        # If the size is a square you can only specify a single number
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(-1, self.num_flat_features(x))
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```

```python
# create your optimizer
optimizer = optim.SGD(net.parameters(), lr=0.01)

# in your training loop:
optimizer.zero_grad()   # zero the gradient buffers
output = net(input)
loss = criterion(output, target)
loss.backward()
optimizer.step()    # Does the update
```

Gradient Descent: $$\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \hat{y}) \qquad \forall l$$

Seems simple enough, why are packages like PyTorch, Tensorflow, Theano, Cafe, MxNet synonymous with deep learning?

1. Automatic differentiation

2. Convenient libraries

3. GPU support

Common training issues

$f_1(f_2(f_3(f_4(x))))$ ← If not careful, this can easily blow up or go to 0.

Neural networks are **non-convex**

- For large networks, **gradients** can **blow up** or **go to zero**. This can be helped by **batchnorm** or ResNet architecture

- **Stepsize**, **batchsize**, **momentum** all have large impact on optimizing the training error *and* generalization performance

- Fancier alternatives to SGD (Adagrad, Adam, LAMB, etc.) can significantly improve training

-Overfitting is common and not undesirable: typical to achieve 100% training accuracy even if test accuracy is just 80%

- Making the network *bigger* may make training *faster!*

- Very important to normalize features & scale weight initialization so that activations throughout network have variance ~1.*

Common training issues

Training is too slow:

- Use larger step sizes, develop step size reduction schedule
- Use GPU resources
- Change batch size
- Use momentum and more exotic optimizers (e.g., Adam)
- Apply batch normalization - CAN HELP w/ * (previous slide)
- Make network larger or smaller (# layers, # filters per layer, etc.)

Test accuracy is low

- Try modifying all of the above, plus changing other hyperparameters

Common training issues

https://playground.tensorflow.org/

Backprop

Matt Golub
Hunter Schafer

UNIVERSITY of WASHINGTON

Backprop

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

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

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

$$\vdots$$

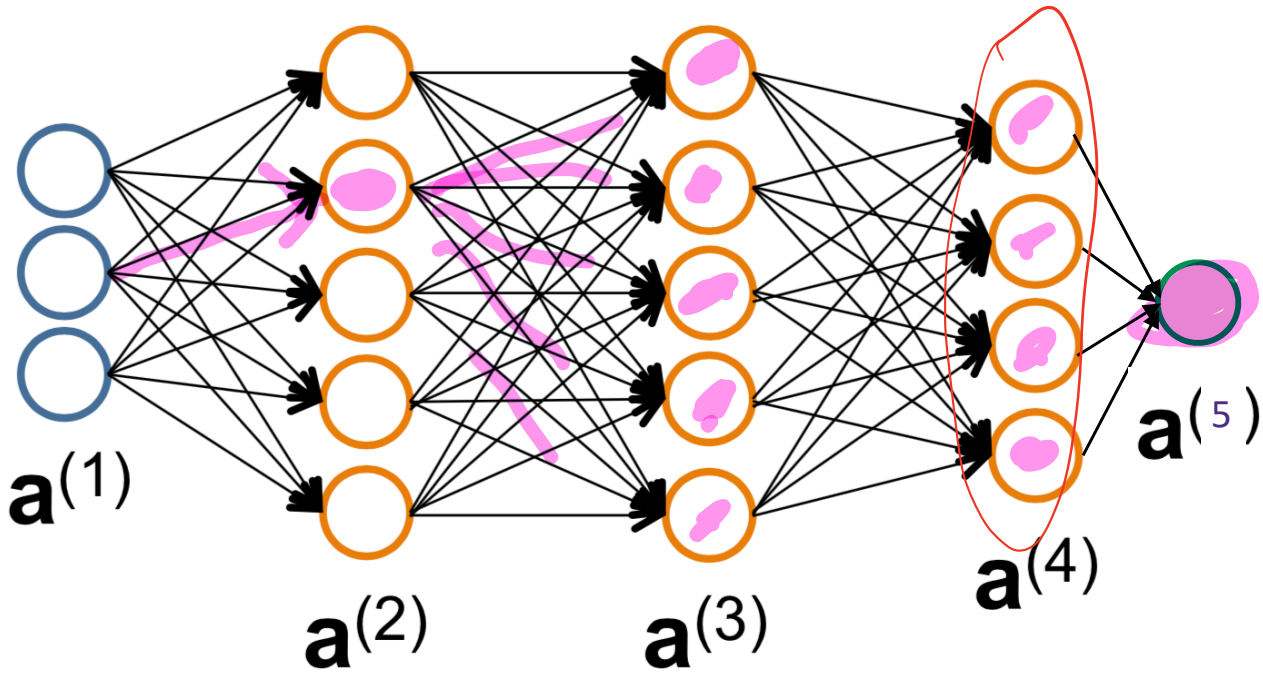
$$a^{(l)} = g\left(z^{(l)}\right)$$

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

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

$$\vdots$$

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



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

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

Backprop

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

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

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

Linear

Non-linearity

$$\vdots$$

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

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

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

$$\vdots$$

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

Train by Stochastic Gradient Descent:

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

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

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

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

Chain Rule:

$h(x) = f(g(x)) \Rightarrow h'(x) = f'(g(x))\, g'(x)$

Also often written as:

Let $u = g(x)$ $\quad \frac{\partial h}{\partial x} = \frac{\partial f}{\partial u} \cdot \frac{\partial u}{\partial x}$

Backprop

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

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

Train by Stochastic Gradient Descent:

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

$z_i^{(l+1)} = \sum_{k=1}^{d} \Theta_{i,k}^{(l)} a_k^{(l)} \quad \frac{\partial z_i^{(l+1)}}{\partial \Theta_{i,j}^{(l)}} = a_j^{(l)}$

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

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

Backprop

$$a^{(1)} = x$$
$$z^{(2)} = \Theta^{(1)} a^{(1)}$$
$$a^{(2)} = g\left(z^{(2)}\right)$$
$$\vdots$$
$$a^{(l)} = g\left(z^{(l)}\right)$$
$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$
$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$
$$\vdots$$
$$\hat{y} = a^{(L+1)}$$

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

Chain rule + Law of total derivatives

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

Definition

$\delta_k^{(l+1)}$

(again, by our definition)

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

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

Backprop

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

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

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

$$\vdots$$

$$a^{(l)} = g(z^{(l)})$$

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

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

$$\vdots$$

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

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

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

Definition

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

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

$$z_k^{(l+1)} = \sum_{m=1}^{d} \Theta_{k,m}^{(l)} g(z_m^{(l)})$$

$$\frac{\partial z_k^{(l+1)}}{\partial z_i^{(l)}} = \Theta_{k,i}^{(l)} g'(z_i^{(l)})$$

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

Special property of Sigmoid

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

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

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

Backprop

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

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

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

$$\vdots$$

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

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

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

$$\vdots$$

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

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

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

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

Recursive Algorithm!

① Push x through. ② Backpropagate δ's.

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

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

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

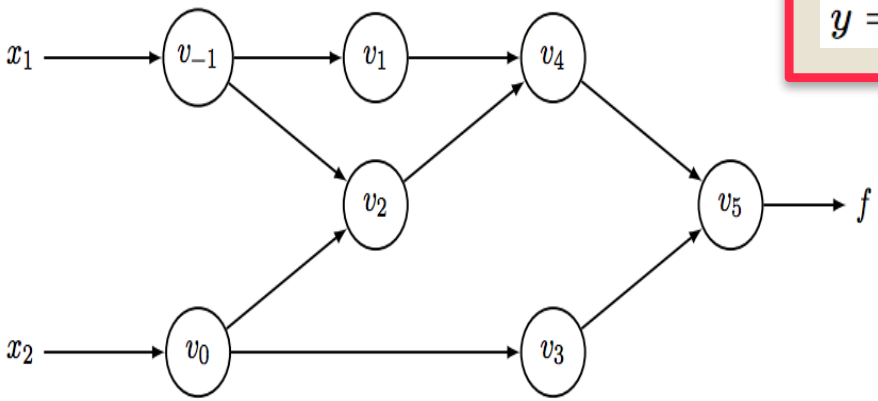
Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

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

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

Autodiff

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



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

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

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

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

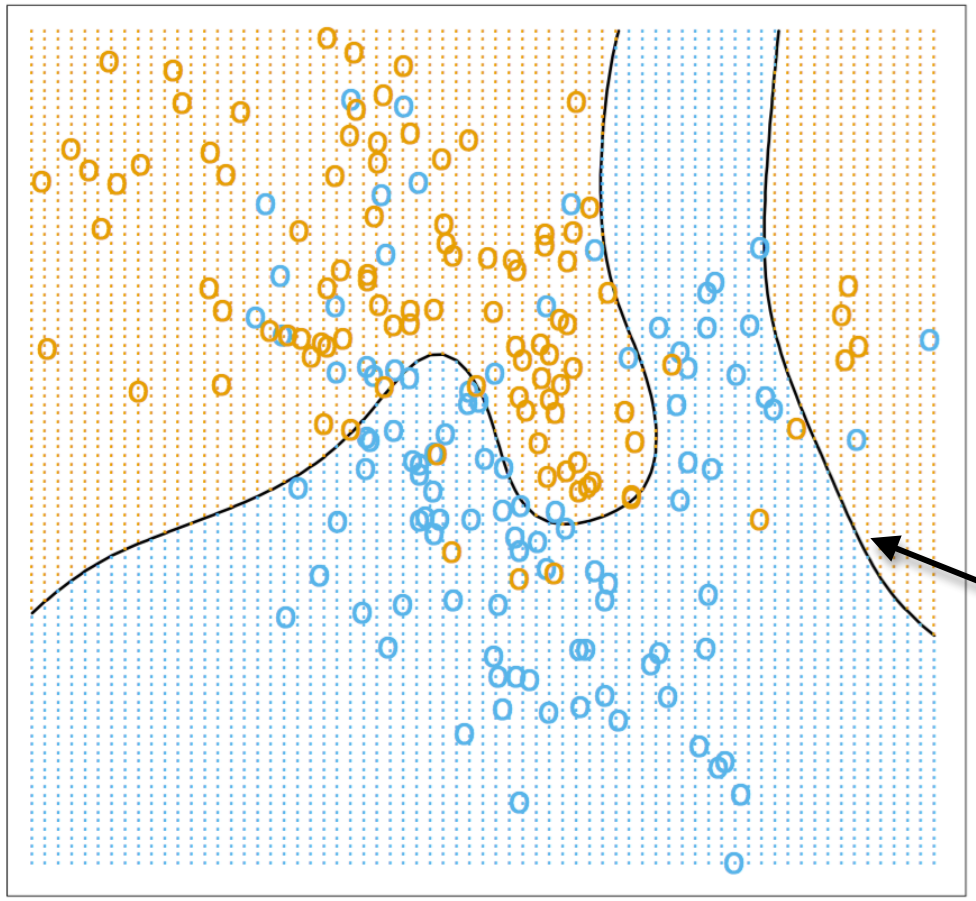
- A model is called “parametric” if the number of parameters do not depend on the number of samples
- A model is called “non-parametric” if the number of parameters increase with the number of samples (Does **not** mean absence of parameters!)

Nearest Neighbor Methods

Matt Golub
Hunter Schafer

UNIVERSITY of WASHINGTON

Some data, Bayes Classifier



Training data:

True label: +1

True label: -1

Optimal "Bayes" classifier:

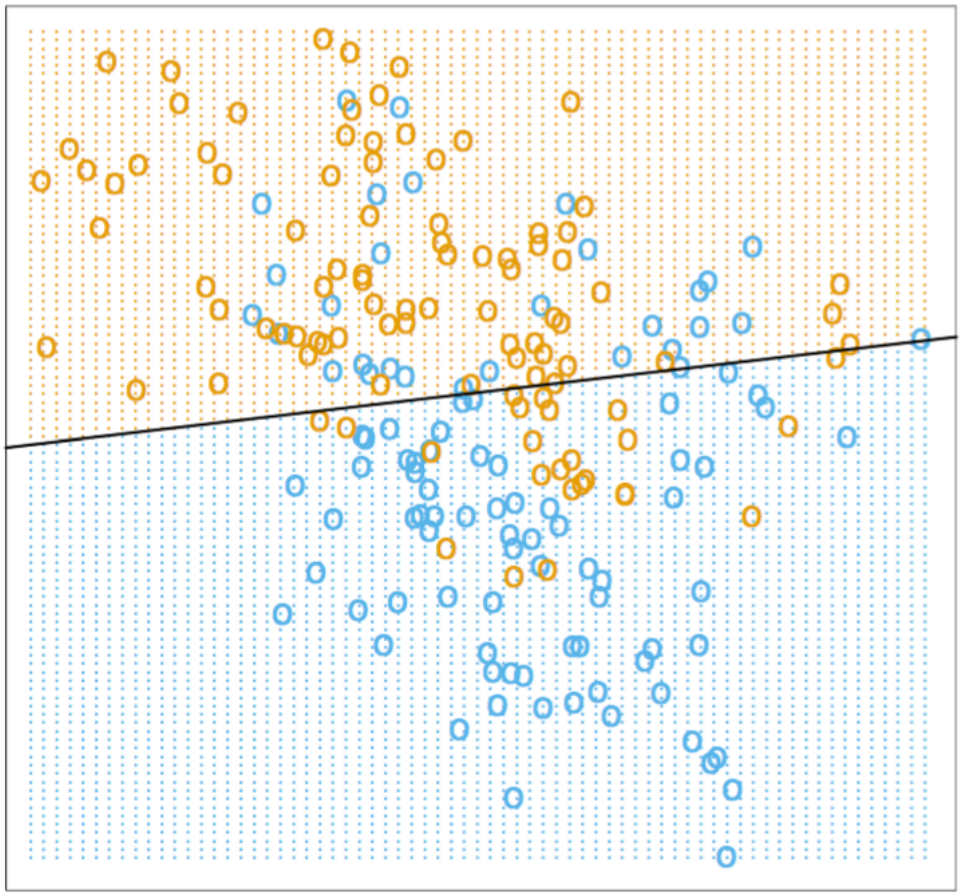
$$\mathbb{P}(Y = 1|X = x) = \frac{1}{2}$$

Predicted label: +1

Predicted label: -1

Figures from Hastie et al.

Linear Decision Boundary



Training data:

True label: +1

True label: -1

Learned:

Linear Decision boundary

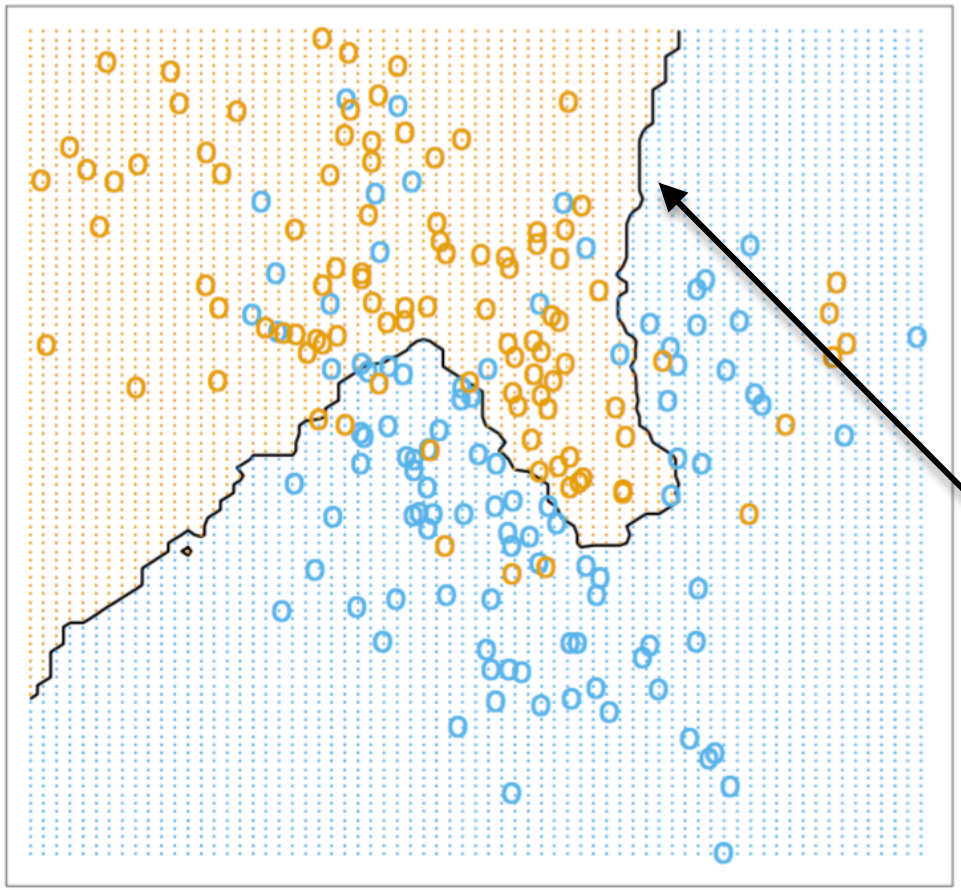
$$x^T w + b = 0$$

Predicted label: +1

Predicted label: -1

Figures from Hastie et al

k=15 Nearest Neighbor Boundary



Training data:

True label: +1

True label: -1

Learned:

15 nearest neighbor decision boundary (majority vote)

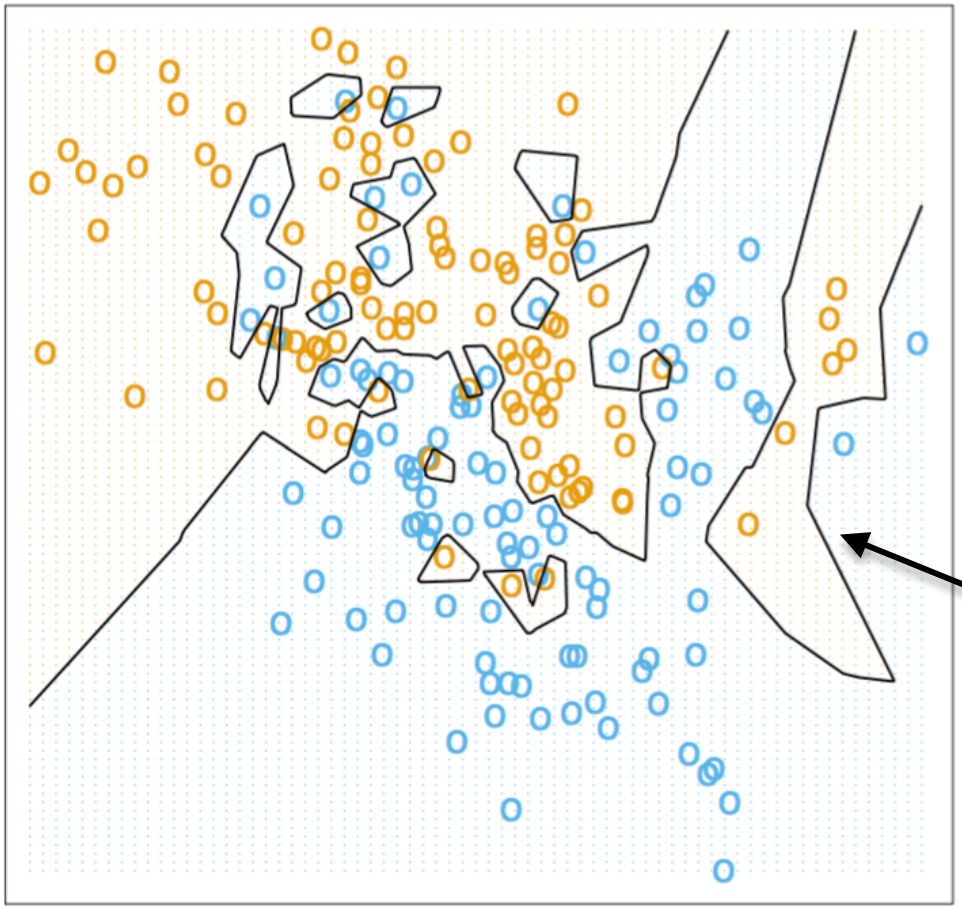
Predicted label: +1

Predicted label: -1

- Nearest neighbor gives non-linear decision boundaries
- What happens if we use a small k or a large k?

Figures from Hastie et al

k=1 Nearest Neighbor Boundary



Training data:

True label: +1

True label: -1

Learned:

1 nearest neighbor decision boundary (majority vote)

Predicted label: +1

Predicted label: -1

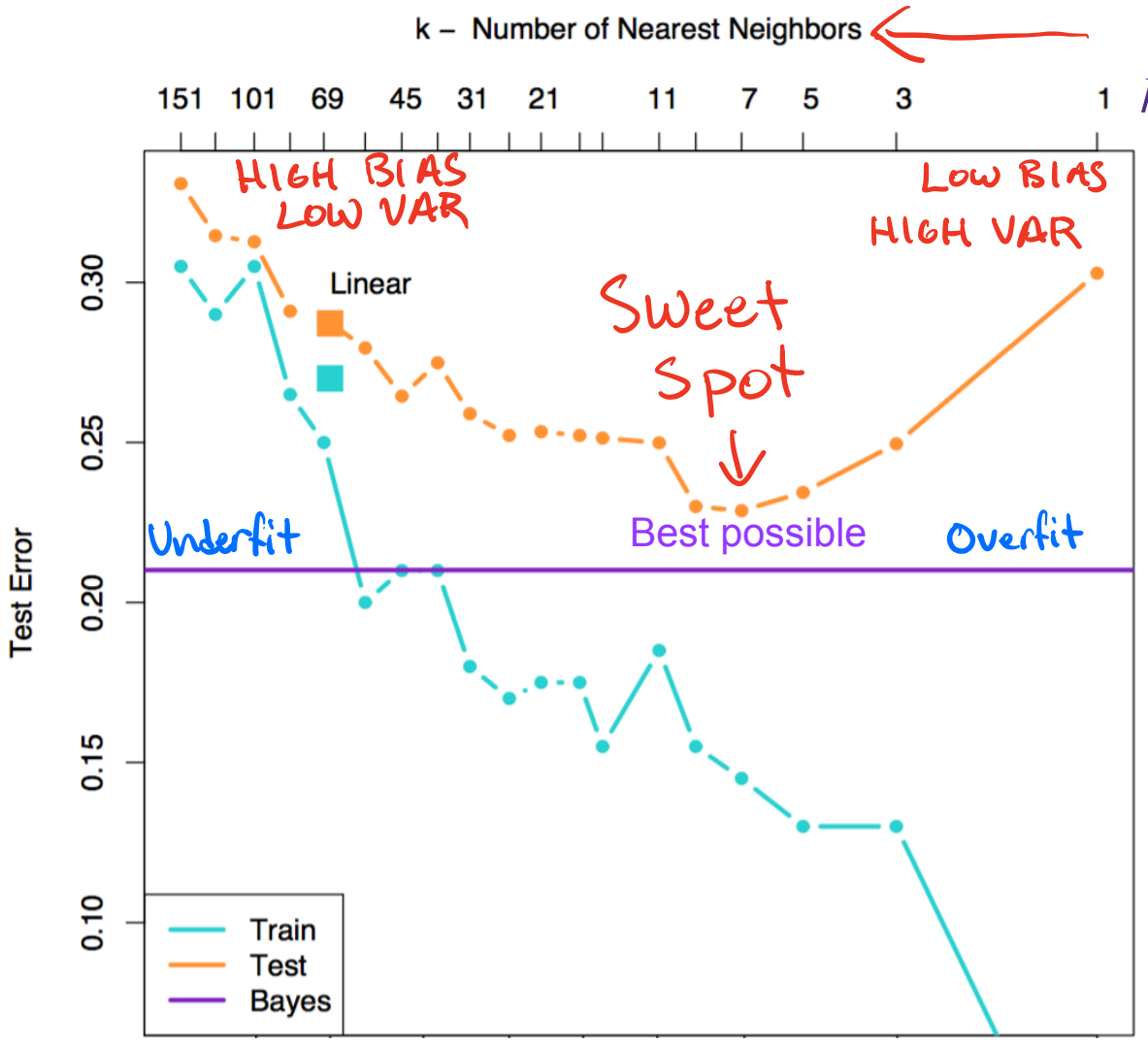
- With a small k, we tend to overfit.

Figures from Hastie et al

k-Nearest Neighbor Error

Model complexity low

Model complexity high



Figures from Hastie et al

Bias-Variance tradeoff

As k->infinity?

Bias: ↑

Variance: ↓

As k->1?

Bias: ↓

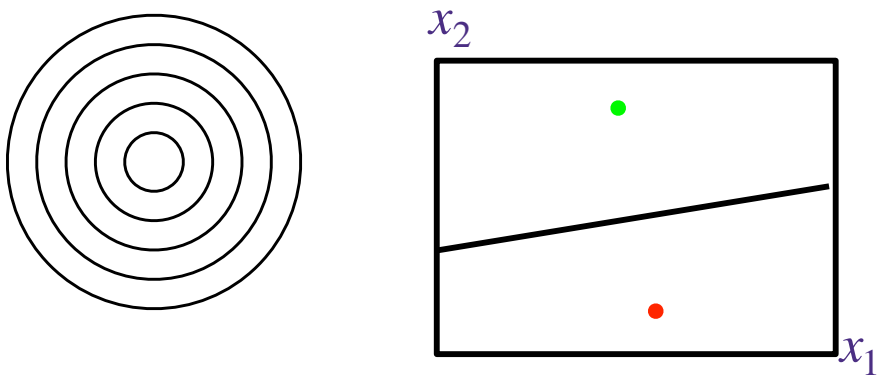
Variance: ↑

- The error achieved by Bayes optimal classifier provides a lower bound on what any estimator can achieve

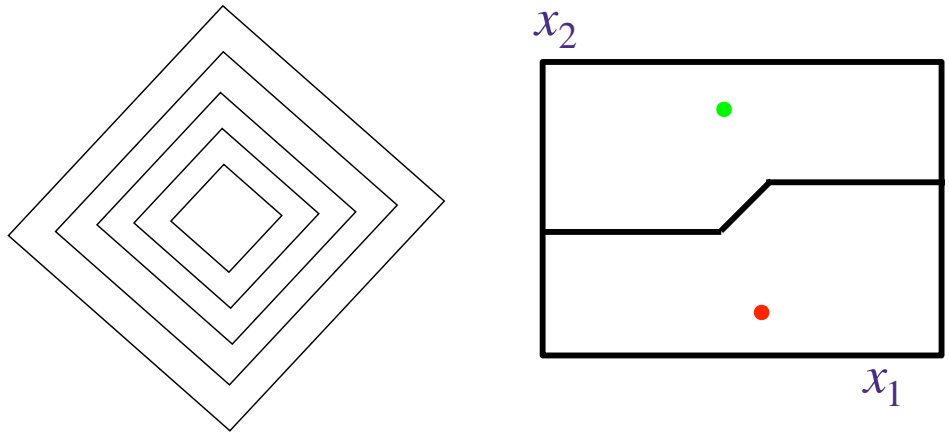
Notable distance metrics (and their level sets)

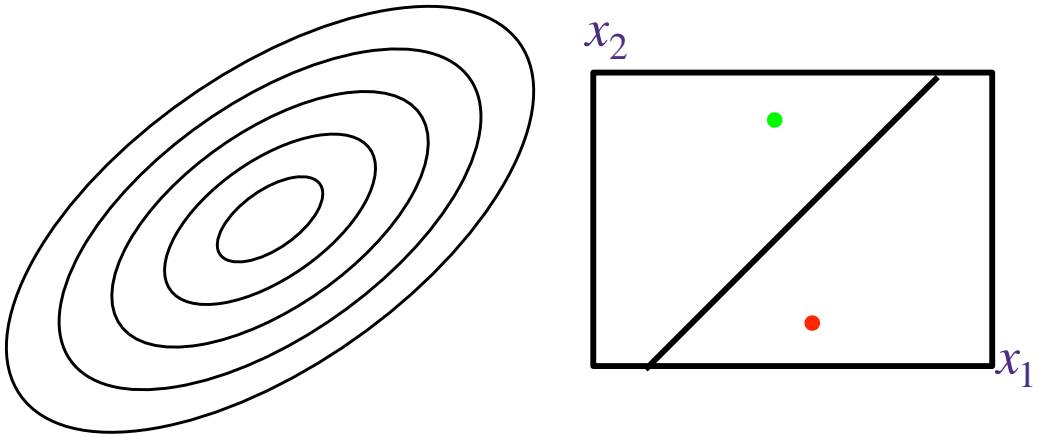
Consider 2 dimensional example with 2 data points with labels green, red,
and we show $k = 1$nearest neighbor decision boundaries for various choices of distances

L_2 norm : $d(x, y) = \|x - y\|_2$

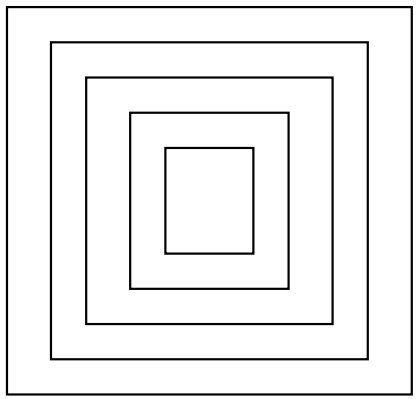


L_1 norm (taxi-cab)

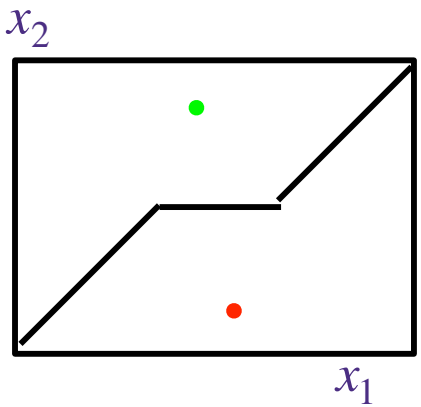




Mahalanobis norm: $d(x, y) = (x - y)^T M (x - y)$

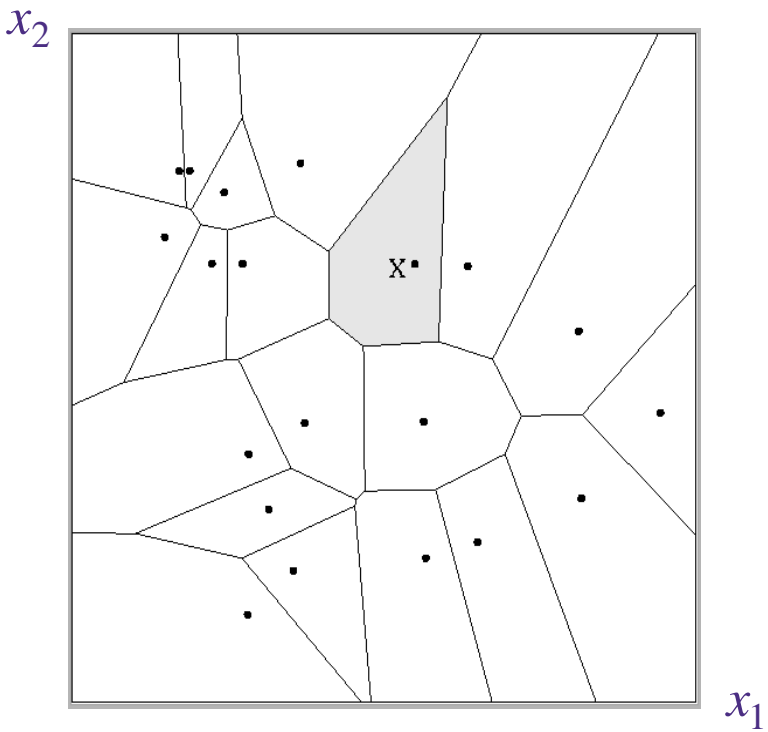


L-infinity *(max) norm*

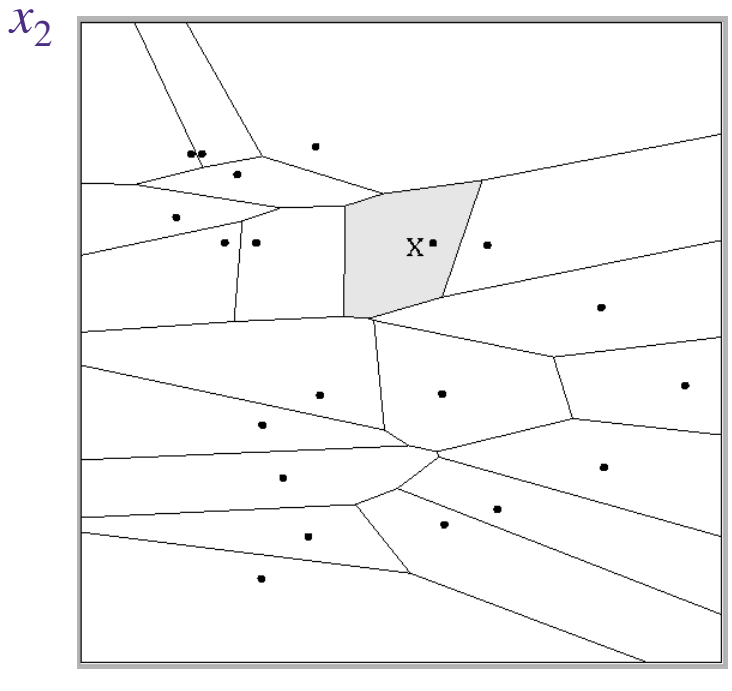


$k = 1$ nearest neighbor

One can draw the nearest-neighbor regions in input space.



$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (x^i_2 - x^j_2)^2$



$Dist(\mathbf{x}^i,\mathbf{x}^j) = (x^i_1 - x^j_1)^2 + (3x^i_2 - 3x^j_2)^2$

The relative scalings in the distance metric affect region shapes

1 nearest neighbor guarantee - classification

$$\{(x_i, y_i)\})_{i=1}^n \qquad x_i \in \mathbb{R}^d, \quad y_i \in \{0, 1\} \qquad (x_i, y_i) \overset{iid}{\sim} P_{XY}$$

Theorem[Cover, Hart, 1967] If P_X is supported everywhere in $\mathbb{R}^d$ and $P(Y = 1|X = x)$ is smooth everywhere, then as $n \to \infty$ the 1-NN classification rule has error at most twice the Bayes error rate.

1 nearest neighbor guarantee - classification

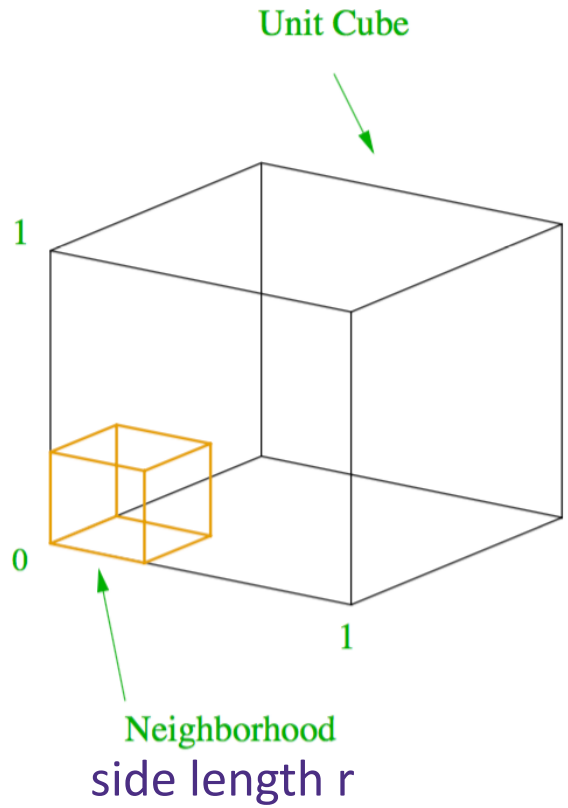
$$\{(x_i, y_i)\})_{i=1}^n \qquad x_i \in \mathbb{R}^d, \quad y_i \in \{0, 1\} \qquad (x_i, y_i) \overset{iid}{\sim} P_{XY}$$

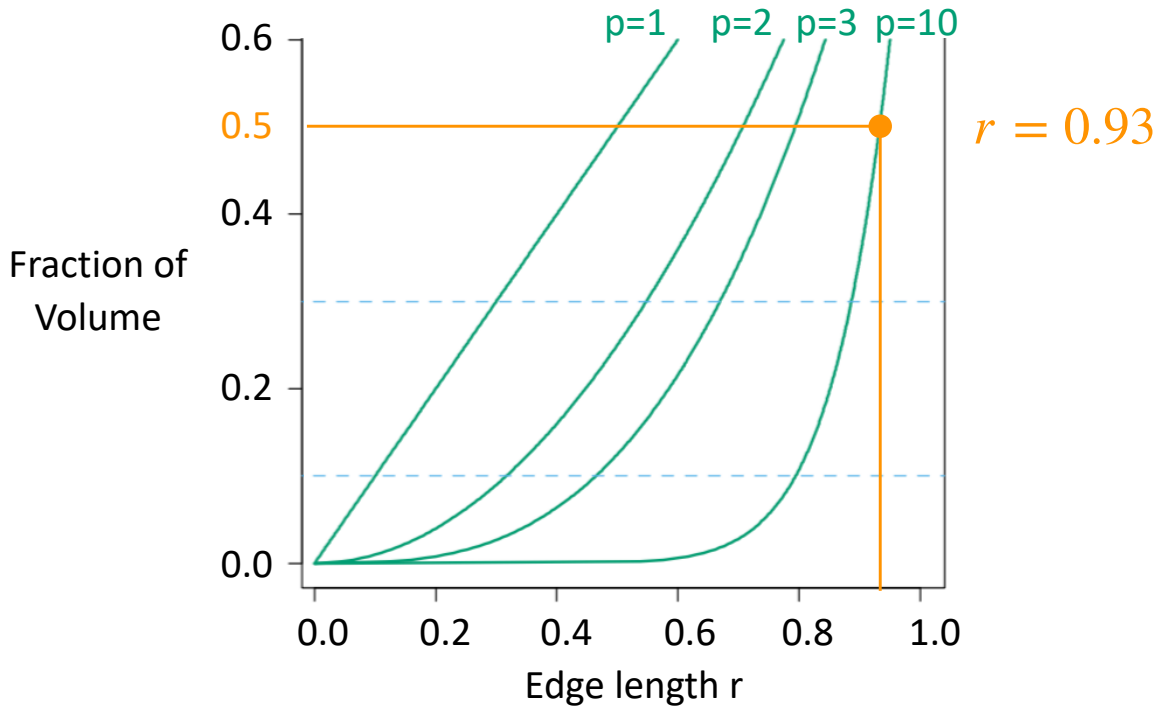
Theorem[Cover, Hart, 1967] If P_X is supported everywhere in $\mathbb{R}^d$ and $P(Y = 1|X = x)$ is smooth everywhere, then as $n \to \infty$ the 1-NN classification rule has error at most twice the Bayes error rate.

- Let x_{NN} denote the nearest neighbor at a point x
- First note that as $n \to \infty, P(y = +1 \,|\, x_{NN}) \to P(y = +1 \,|\, x)$
- Let $p^* = \min\{P(y = +1 \,|\, x), P(y = -1 \,|\, x)\}$ denote the Bayes error rate
- At a point x,
  - Case 1: nearest neighbor is $+1$, which happens with $P(y = +1 \,|\, x)$ and the error rate is $P(y = -1 \,|\, x)$
  - Case 2: nearest neighbor is -1, which happens with $P(y = -1 \,|\, x)$ and the error rate is $P(y = +1 \,|\, x)$
- The average error of a 1-NN is

$$P(y = +1 \,|\, x)\, P(y = -1 \,|\, x) + P(y = -1 \,|\, x)\, P(y = +1 \,|\, x) \;= 2p^*(1 - p^*)$$

Curse of dimensionality Ex. 1



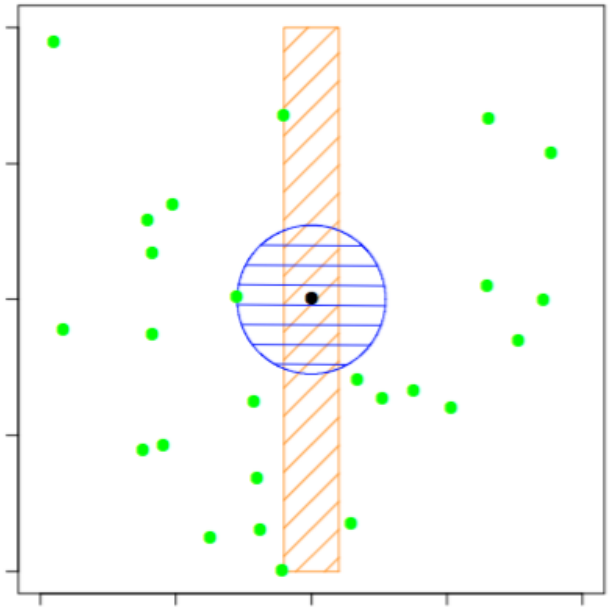


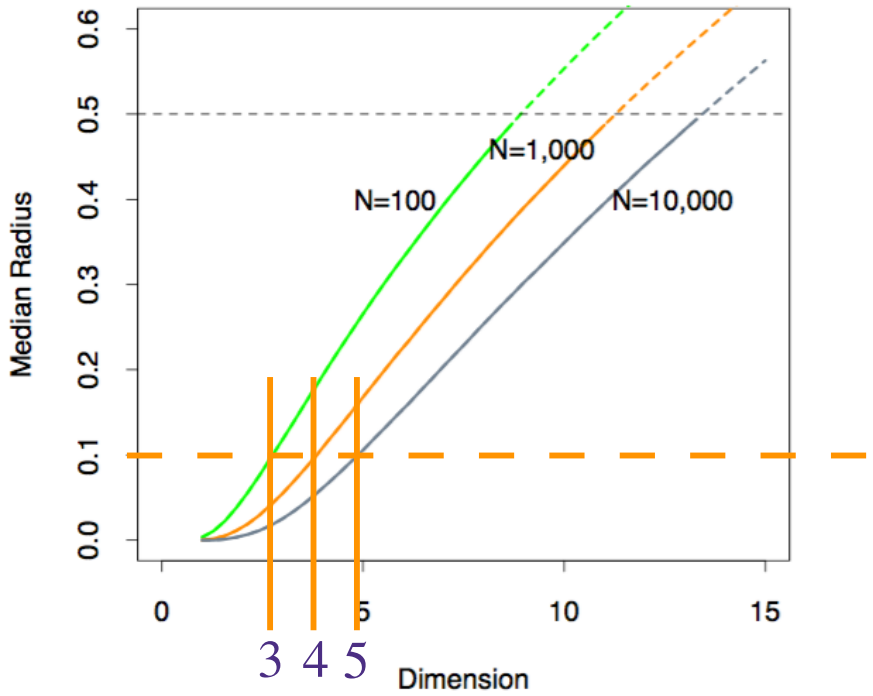
X is uniformly distributed over $[0,1]^p$. What is $\mathbb{P}(X \in [0,r]^p)$?

How many samples do we need so that a nearest neighbor is within a cube of side length r?

Curse of dimensionality Ex. 2

$\{X_i\}_{i=1}^n$ are uniformly distributed over $[-.5, .5]^p$.

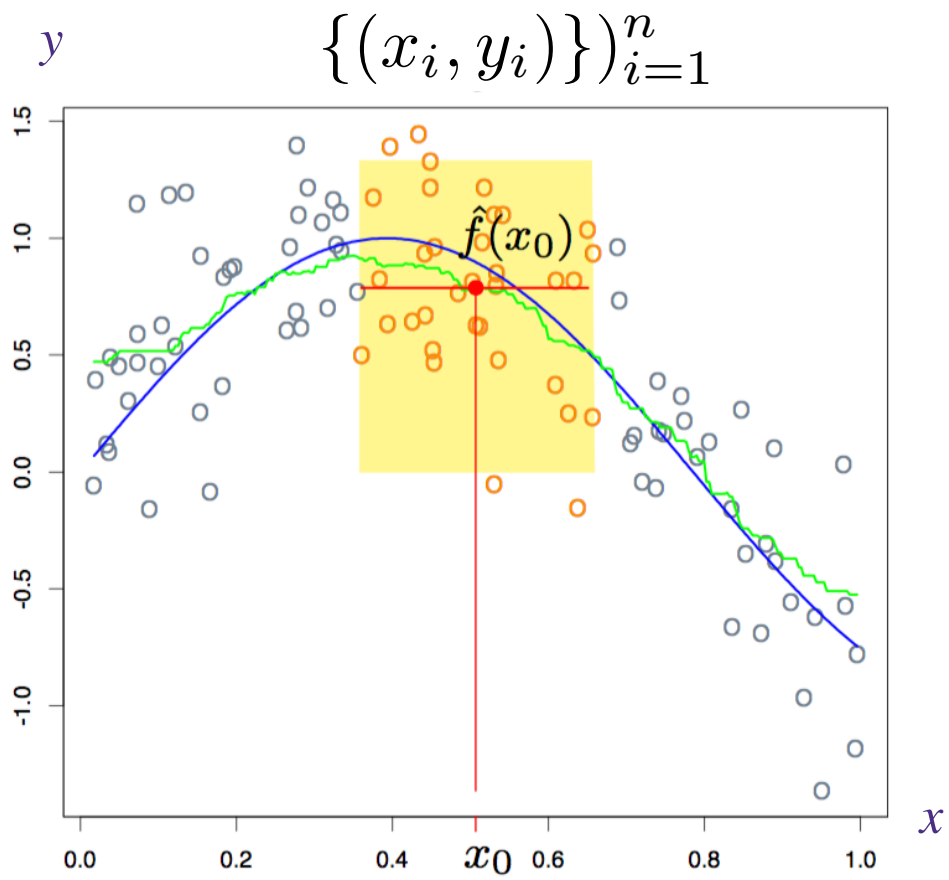




What is the median distance from a point at origin to its 1NN?

How many samples do we need so that a median Euclidean distance is within r?

Nearest neighbor regression



- What is the optimal classifier that minimizes MSE $\mathbb{E}[(\hat{y} - y)^2]$?

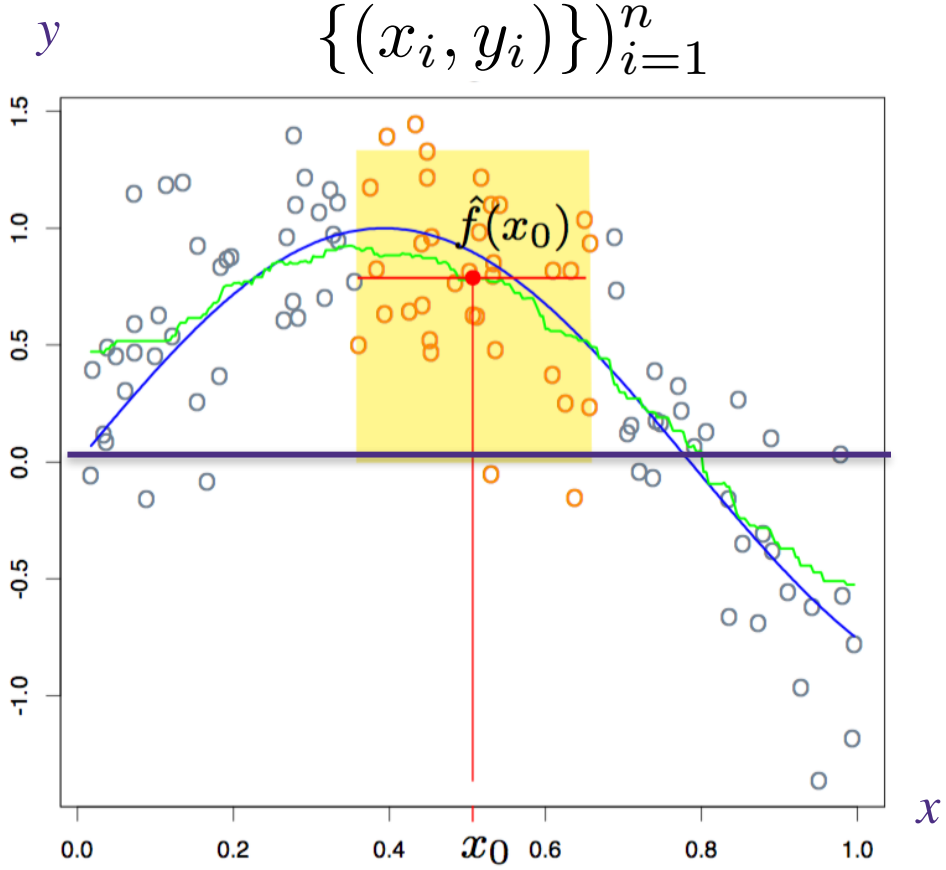
$$\hat{y} = \mathbb{E}[y \mid x]$$

- k-nearest neighbor regressor is

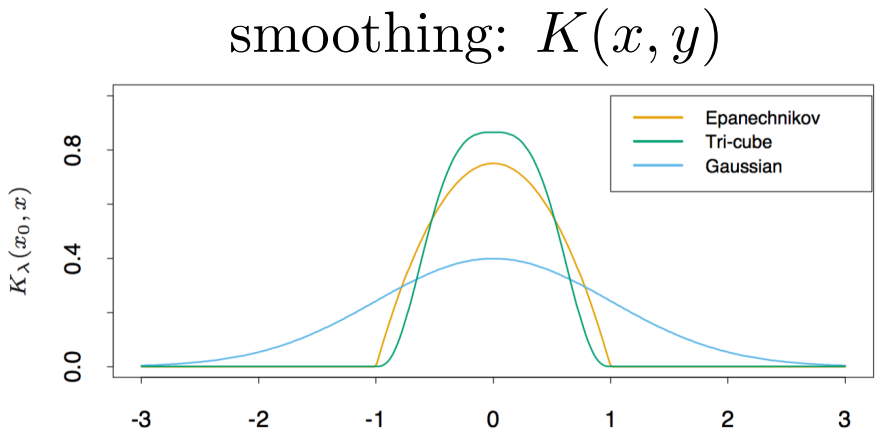
$$\hat{f}(x) = \frac{1}{k} \sum_{j \in \text{nearest neighbor}} y_j$$

$$= \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

Nearest neighbor regression



In nearest neighbor methods, the "weight" changes abruptly

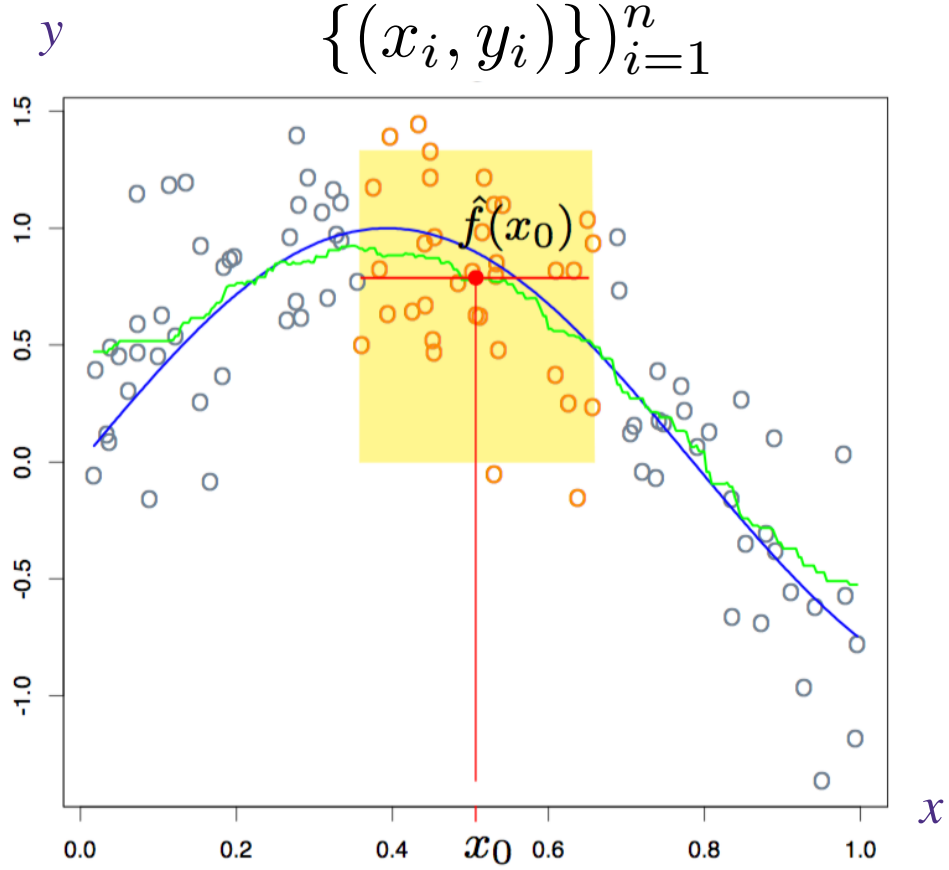


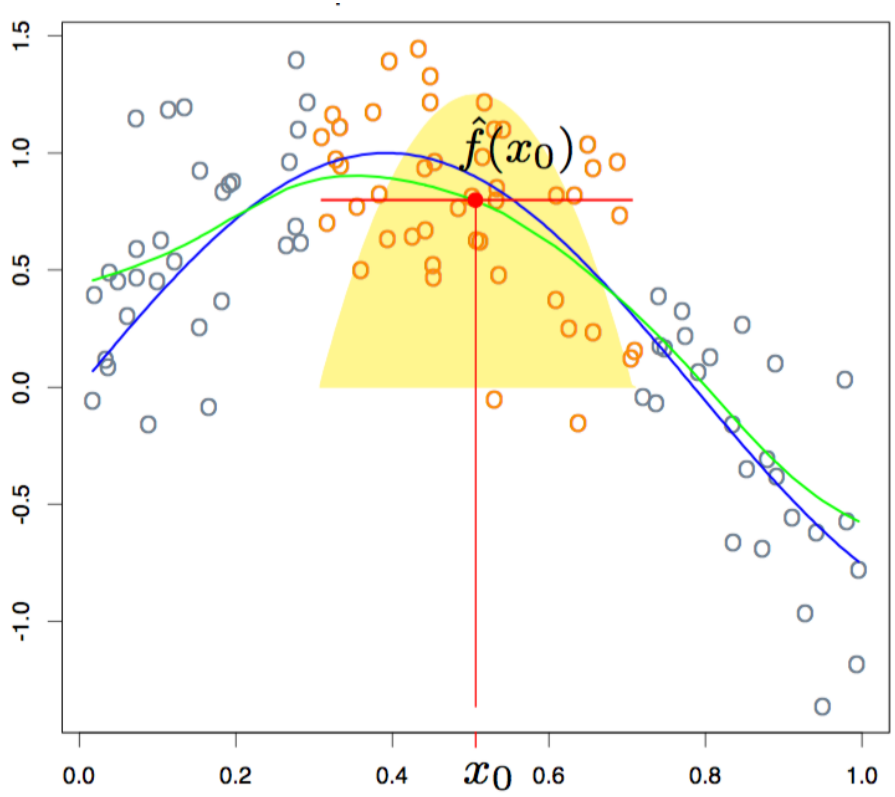
- k-nearest neighbor regressor is

$$\hat{f}(x_0) = \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

Nearest neighbor regression



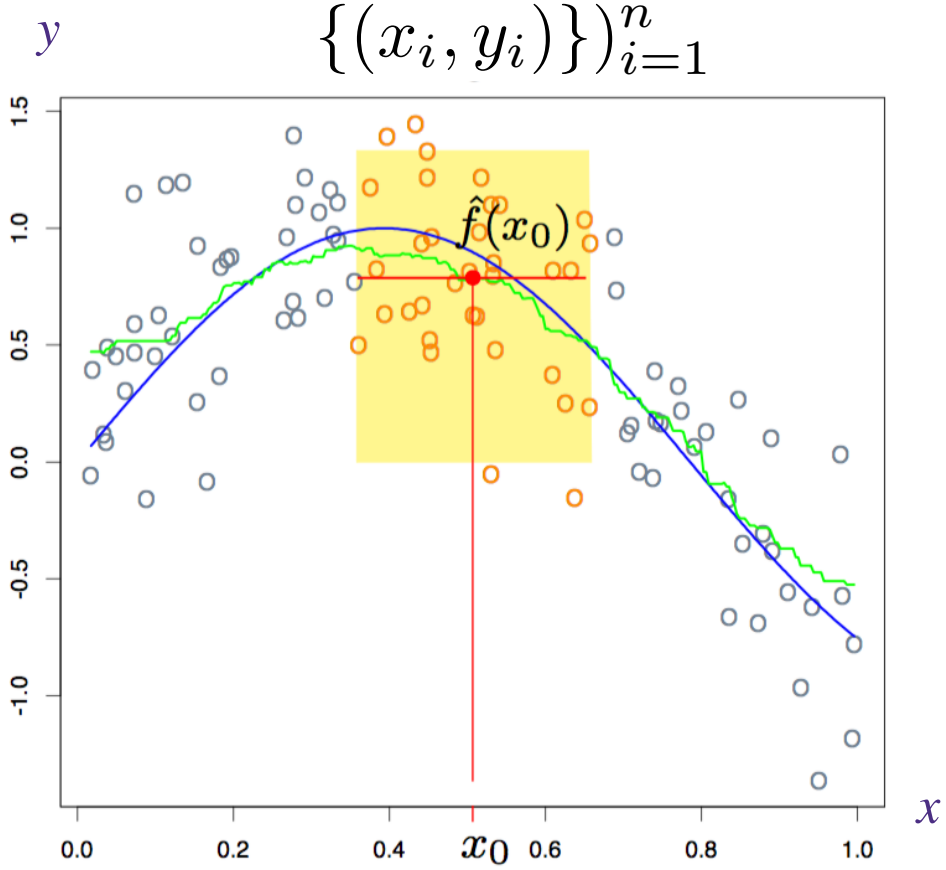


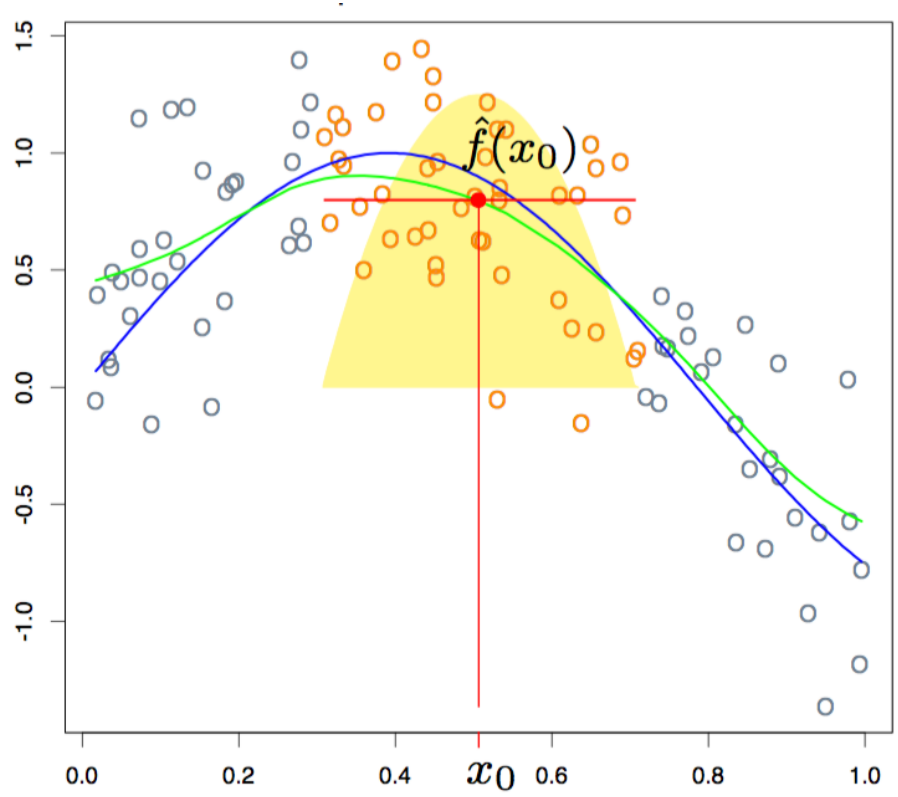
- k-nearest neighbor regressor is

$$\hat{f}(x_0) = \frac{\sum_{i=1}^{n} y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^{n} \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^{n} K(x_0, x_i) y_i}{\sum_{i=1}^{n} K(x_0, x_i)}$$

Nearest neighbor regression





Why just average them?

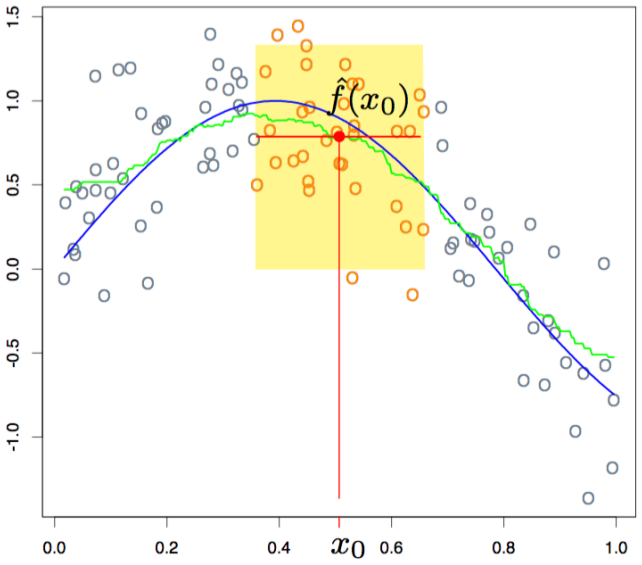
- k-nearest neighbor regressor is

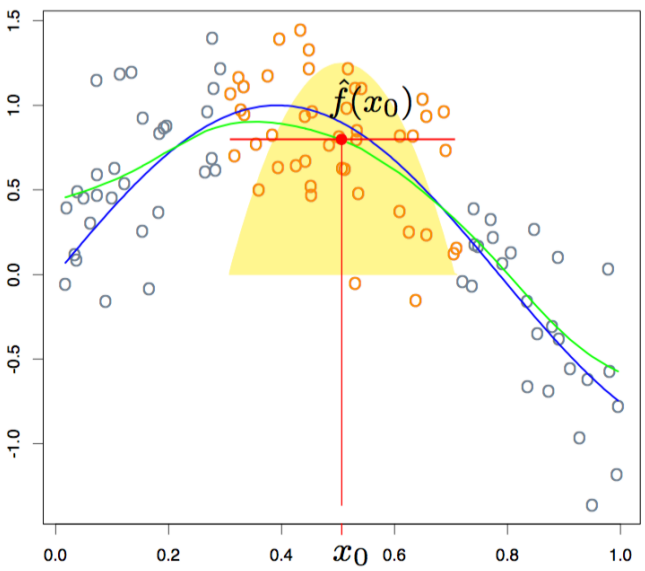
$$\hat{f}(x_0) = \frac{\sum_{i=1}^{n} y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^{n} \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

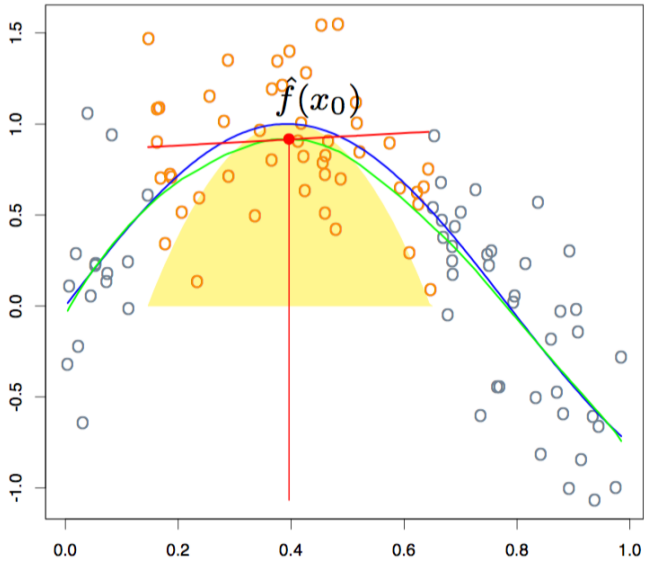
$$\widehat{f}(x_0) = \frac{\sum_{i=1}^{n} K(x_0, x_i) y_i}{\sum_{i=1}^{n} K(x_0, x_i)}$$

Nearest neighbor regression

$$\{(x_i, y_i)\})_{i=1}^n$$







- k-nearest neighbor regressor is

$$\hat{f}(x_0) = \frac{\sum_{i=1}^n y_i \times \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}{\sum_{i=1}^n \text{Ind}(x_i \text{ is a } k \text{ nearest neighbor})}$$

$$\widehat{f}(x_0) = \frac{\sum_{i=1}^n K(x_0, x_i) y_i}{\sum_{i=1}^n K(x_0, x_i)}$$

$$\widehat{f}(x_0) = b(x_0) + w(x_0)^T x_0$$

$$w(x_0), b(x_0) = \arg\min_{w,b} \sum_{i=1}^n K(x_0, x_i)(y_i - (b + w^T x_i))^2$$

Local Linear Regression

Nearest Neighbor Overview

- Very simple to explain and implement
- No training! But finding nearest neighbors in large dataset at test can be computationally demanding (KD-trees help)
- You can use other forms of distance (not just Euclidean)
- Smoothing and local linear regression can improve performance (at the cost of higher variance)
- With a lot of data, “local methods” have strong, simple theoretical guarantees.
- Without a lot of data, neighborhoods aren’t “local” and methods suffer (curse of dimensionality).

Questions?