CSCE 478/878 Lecture 4: Artificial Neural Networks

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(Adapted from Tom Mitchell's slides)

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Outline

- Threshold units: Perceptron, Winnow
- Gradient descent/exponentiated gradient
- Multilayer networks
- Backpropagation
- Advanced topics
- Support Vector Machines

Connectionist Models

Consider humans:

- Total number of neurons $\approx 10^{10}$
- Neuron switching time $\approx 10^{-3}$ second (vs. 10^{-10})
- Connections per neuron $\approx 10^4$–10^5
- Scene recognition time ≈ 0.1 second
- 100 inference steps doesn't seem like enough

$\Rightarrow$ much parallel computation

Properties of artificial neural nets (ANNs):

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process
- Emphasis on tuning weights automatically

Strong differences between ANNs for ML and ANNs for biological modeling

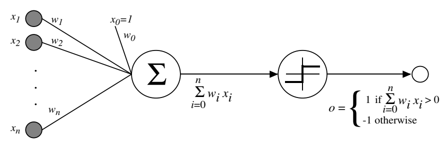
When to Consider Neural Networks

- Input is high-dimensional discrete- or real-valued (e.g. raw sensor input)
- Output is discrete- or real-valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant
- Long training times acceptable

Examples:

- Speech phoneme recognition [Waibel]
- Image classification [Kanade, Baluja, Rowley]
- Financial prediction

The Perceptron & Winnow



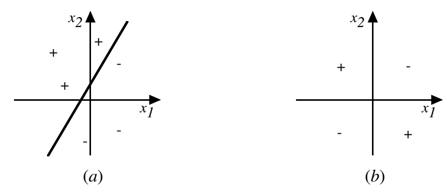
$$o(x_1, \ldots, x_n) = \begin{cases} +1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise} \end{cases}$$

(sometimes use 0 instead of -1)

Sometimes we'll use simpler vector notation:

$$o(\vec{x}) = \begin{cases} +1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\ -1 & \text{otherwise} \end{cases}$$

Decision Surface of Perceptron/Winnow



Represents some useful functions

- What weights represent $g(x_1, x_2) = AND(x_1, x_2)$?

But some functions not representable

- I.e. those not linearly separable
- Therefore, we'll want networks of neurons

Perceptron Training Rule

$$w_i \leftarrow w_i + \Delta w_i^{add}, \text{ where } \Delta w_i^{add} = \eta(t-o)x_i$$

and

- $t = c(\vec{x})$ is target value
- o is perceptron output
- η is small constant (e.g. 0.1) called learning rate

I.e. if $(t-o) > 0$ then increase w_i w.r.t. x_i, else decrease

Can prove rule will converge if training data is linearly separable and η sufficiently small

Winnow Training Rule

$$w_i \leftarrow w_i \cdot \Delta w_i^{mult}, \text{ where } \Delta w_i^{mult} = \alpha^{(t-o)x_i}$$

and $\alpha > 1$

I.e. use multiplicative updates vs. additive updates

Problem: Sometimes negative weights are required

- Maintain two weight vectors $\vec{w}^+$ and $\vec{w}^-$ and replace $\vec{w} \cdot \vec{x}$ with $\left(\vec{w}^+ - \vec{w}^-\right) \cdot \vec{x}$
- Update $\vec{w}^+$ and $\vec{w}^-$ independently as above, using $\Delta w_i^+ = \alpha^{(t-o)x_i}$ and $\Delta w_i^- = 1/\Delta w_i^+$

Can also guarantee convergence

Perceptron vs. Winnow

Winnow works well when most attributes irrelevant, i.e. when optimal weight vector $\vec{w}^*$ is sparse (many 0 entries)

E.g. let examples $\vec{x} \in \{0,1\}^n$ be labeled by a k-disjunction over n attributes, $k \ll n$

- Remaining $n-k$ are irrelevant
- E.g. $c(x_1, \ldots, x_{150}) = x_5 \vee x_9 \vee \neg x_{12}$, $n = 150$, $k = 3$
- For disjunctions, number of prediction mistakes (in on-line model) is $O(k \log n)$ for Winnow and (in worst case) $\Omega(kn)$ for Perceptron
- So in worst case, need exponentially fewer updates for learning with Winnow than Perceptron

Bound is only for disjunctions, but improvement for learning with irrelevant attributes is often true

When $\vec{w}^*$ not sparse, sometimes Perceptron better

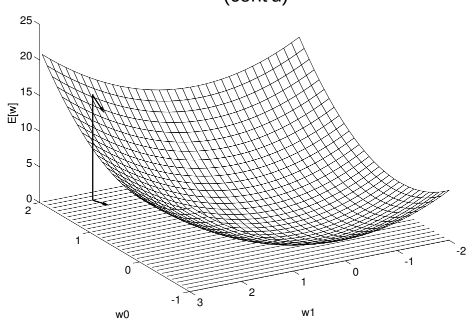
Also, have proofs for agnostic error bounds for both algorithms

Gradient Descent and Exponentiated Gradient

- Useful when linear separability impossible but still want to minimize training error
- Consider simpler *linear unit*, where
  $$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$
  (i.e. no threshold)
- For moment, assume that we update weights after seeing each example $\vec{x}_d$
- For each example, want to compromise between correctiveness and conservativeness
  - Correctiveness: Tendency to improve on $\vec{x}_d$ (reduce error)
  - Conservativeness: Tendency to keep $\vec{w}_{d+1}$ close to $\vec{w}_d$ (minimize distance)
- Use cost function that measures both:

$$U(\vec{w}) = dist\left(\vec{w}_{d+1}, \vec{w}_d\right) + \eta\, error\left(t_d, \overbrace{\vec{w}_{d+1} \cdot \vec{x}_d}^{\text{curr ex, new wts}}\right)$$

Gradient Descent and Exponentiated Gradient (cont'd)



$$\frac{\partial U}{\partial \vec{w}} = \left[\frac{\partial U}{\partial w_0}, \frac{\partial U}{\partial w_1}, \cdots, \frac{\partial U}{\partial w_n}\right]$$

Gradient Descent

$$\begin{aligned} U(\vec{w}) &= \overbrace{\|\vec{w}_{d+1} - \vec{w}_d\|_2^2}^{conserv.} + \overbrace{\eta}^{coef.} \overbrace{(t_d - \vec{w}_{d+1} \cdot \vec{x}_d)^2}^{corrective} \\ &= \sum_{i=1}^{n} \left(w_{i,d+1} - w_{i,d}\right)^2 + \eta \left(t_d - \sum_{i=1}^{n} w_{i,d+1}\, x_{i,d}\right)^2 \end{aligned}$$

Take gradient w.r.t. $\vec{w}_{d+1}$ and set to $\vec{0}$:

$$0 = 2\left(w_{i,d+1} - w_{i,d}\right) - 2\eta \left(t_d - \sum_{i=1}^{n} w_{i,d+1}\, x_{i,d}\right) x_{i,d}$$

Approximate with

$$0 = 2\left(w_{i,d+1} - w_{i,d}\right) - 2\eta \left(t_d - \sum_{i=1}^{n} w_{i,d}\, x_{i,d}\right) x_{i,d} \ ,$$

which yields

$$w_{i,d+1} = w_{i,d} + \overbrace{\eta\,(t_d - o_d)\, x_{i,d}}^{\Delta w_{i,d}^{add}}$$

Exponentiated Gradient

Conserv. portion uses unnormalized relative entropy:

$$U(\vec{w}) = \overbrace{\sum_{i=1}^{n} \left(w_{i,d} - w_{i,d+1} + w_{i,d+1} \ln \frac{w_{i,d+1}}{w_{i,d}} \right)}^{conserv.} + \overbrace{\eta}^{coef.} \overbrace{(t_d - \vec{w}_{d+1} \cdot \vec{x}_d)^2}^{corrective}$$

Take gradient w.r.t. $\vec{w}_{d+1}$ and set to $\vec{0}$:

$$0 = \ln \frac{w_{i,d+1}}{w_{i,d}} - 2\eta \left(t_d - \sum_{i=1}^{n} w_{i,d+1}\, x_{i,d} \right) x_{i,d}$$

Approximate with

$$0 = \ln \frac{w_{i,d+1}}{w_{i,d}} - 2\eta \left(t_d - \sum_{i=1}^{n} w_{i,d}\, x_{i,d} \right) x_{i,d},$$

which yields (for $\eta = \ln \alpha / 2$)

$$w_{i,d+1} = w_{i,d} \exp\left(2\eta \left(t_d - o_d\right) x_{i,d}\right) = w_{i,d}\, \overbrace{\alpha^{(t_d - o_d) x_{i,d}}}^{\Delta w_{i,d}^{mult}}$$

Implementation Approaches

- Can use rules on previous slides on an example-by-example basis, sometimes called incremental, stochastic, or on-line GD/EG
  - Has a tendency to "jump around" more in searching, which helps avoid getting trapped in local minima
- Alternatively, can use standard or batch GD/EG, in which the classifier is evaluated over all training examples, summing the error, and then updates are made
  - I.e. sum up Δw_i for all examples, but don't update w_i until summation complete (p. 93, Table 4.1)
  - This is an inherent averaging process and tends to give better estimate of the gradient

Remarks

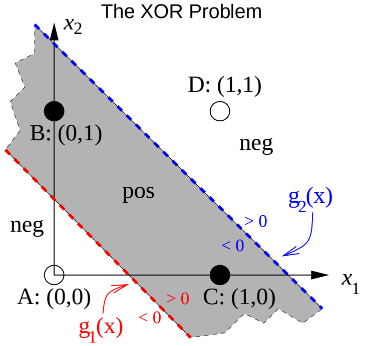
- Perceptron and Winnow update weights based on thresholded output, while GD and EG use unthresholded outputs
- P/W converge in finite number of steps to perfect hyp if data linearly separable; GD/EG work on non-linearly separable data, but only converge asymptotically (to wts with minimum squared error)
- As with P vs. W, EG tends to work better than GD when many attributes are irrelevant
  - Allows the addition of attributes that are nonlinear combinations of original ones, to work around linear sep. problem (perhaps get linear separability in new, higher-dimensional space)
  - E.g. if two attributes are x_1 and x_2, use as EG inputs

$$\vec{x} = \left[x_1, x_2, x_1 x_2, x_1^2, x_2^2\right]$$

- Also, both have provable agnostic results

Handling Nonlinearly Separable Data

The XOR Problem



- Can't represent with a single linear separator, but can with intersection of two:

$$g_1(\vec{x}) = 1 \cdot x_1 + 1 \cdot x_2 - 1/2$$
$$g_2(\vec{x}) = 1 \cdot x_1 + 1 \cdot x_2 - 3/2$$

$$\text{pos} = \left\{\vec{x} \in \Re^{\ell} : g_1(\vec{x}) > 0 \text{ AND } g_2(\vec{x}) < 0\right\}$$

$$\text{neg} = \left\{\vec{x} \in \Re^{\ell} : g_1(\vec{x}), g_2(\vec{x}) < 0 \text{ OR } g_1(\vec{x}), g_2(\vec{x}) > 0\right\}$$

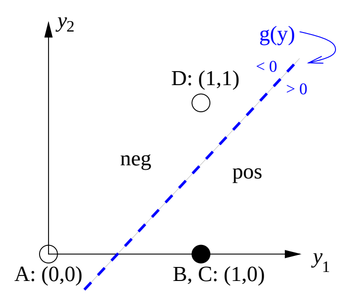
The XOR Problem
(cont'd)

- Let $y_i = \begin{cases} 0 & \text{if } g_i(\vec{x}) < 0 \\ 1 & \text{otherwise} \end{cases}$

Class	(x_1, x_2)	$g_1(\vec{x})$	y_1	$g_2(\vec{x})$	y_2
pos	B: $(0,1)$	$1/2$	1	$-1/2$	0
pos	C: $(1,0)$	$1/2$	1	$-1/2$	0
neg	A: $(0,0)$	$-1/2$	0	$-3/2$	0
neg	D: $(1,1)$	$3/2$	1	$1/2$	1

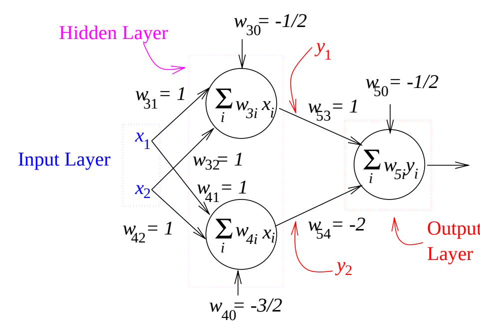
- Now feed y_1, y_2 into:

$$g(\vec{y}) = 1 \cdot y_1 - 2 \cdot y_2 - 1/2$$



The XOR Problem
(cont'd)

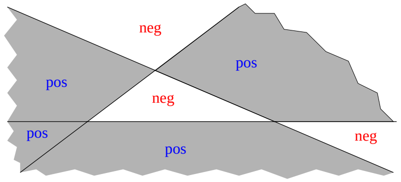
- In other words, we remapped all vectors $\vec{x}$ to $\vec{y}$ such that the classes are linearly separable in the new vector space



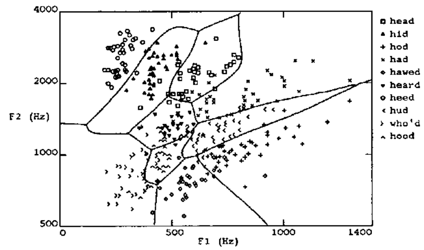
- This is a two-layer perceptron or two-layer feedforward neural network
- Each neuron outputs 1 if its weighted sum exceeds its threshold, 0 otherwise

Generally Handling Nonlinearly Separable Data

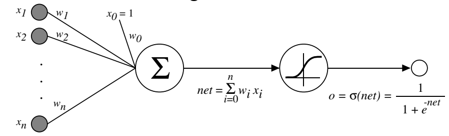
- By adding up to 2 hidden layers of perceptrons, can represent any union of intersection of halfspaces



- Problem: The above is still defined linearly



Sigmoid Unit



$\sigma(x)$ is the logistic function

$$\frac{1}{1+e^{-x}}$$

(a type of sigmoid function)

Squashes net into $[0, 1]$ range

Nice property:

$$\frac{d\sigma(x)}{dx} = \sigma(x)(1-\sigma(x))$$

We can derive GD/EG rules to train

- One sigmoid unit
- *Multilayer networks* of sigmoid units $\Rightarrow$ Backpropagation

GD/EG for Sigmoid Unit

- First note that conservativeness and correctiveness are only additively related $\Rightarrow$ derivatives always independent
- Thus in general get

$$w_{i,d+1} = w_{i,d} - \frac{\eta}{2}\frac{\partial\, correc}{\partial w_{i,d}} \quad \text{for GD}$$

$$w_{i,d+1} = w_{i,d} \exp\left(-\eta \frac{\partial\, correc}{\partial w_{i,d}}\right) \quad \text{for EG}$$

- So all we have to do is define an error function, take its gradient, and substitute into the equations

GD/EG for Sigmoid Unit
(cont'd)

Return to book notation, where correctiveness is:

$$E(\vec{w}_d) = \frac{1}{2}(t_d - o_d)^2$$

(folding $1/2$ of correctiveness into error func)

Thus $\frac{\partial E}{\partial w_{i,d}} = \frac{\partial}{\partial w_{i,d}} \frac{1}{2}(t_d - o_d)^2$

$$= \frac{1}{2} 2 (t_d - o_d) \frac{\partial}{\partial w_{i,d}} (t_d - o_d) = (t_d - o_d)\left(-\frac{\partial o_d}{\partial w_{i,d}}\right)$$

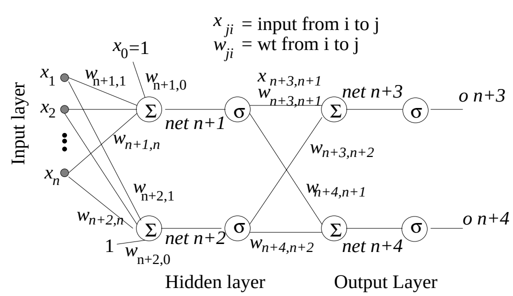
Since o_d is a function of $net_d = \vec{w}_d \cdot \vec{x}_d$,

$$\begin{aligned}\frac{\partial E}{\partial w_{i,d}} &= -(t_d - o_d)\frac{\partial o_d}{\partial net_d}\frac{\partial net_d}{\partial w_{i,d}} \\ &= -(t_d - o_d)\frac{\partial \sigma(net_d)}{\partial net_d}\frac{\partial net_d}{\partial w_{i,d}} \\ &= -(t_d - o_d)\, o_d\, (1 - o_d)\, x_{i,d}\end{aligned}$$

$$\boxed{w_{i,d+1} = w_{i,d} + \eta\, o_d\, (1 - o_d)\, (t_d - o_d)\, x_{i,d} \quad \text{for GD}}$$

$$\boxed{w_{i,d+1} = w_{i,d} \exp\left(2\eta\, o_d\, (1 - o_d)\, (t_d - o_d)\, x_{i,d}\right) \quad \text{for EG}}$$

Multilayer Networks



Use sigmoid units since continuous and differentiable

Error:

$$E_d = E(\vec{w}_d) = \frac{1}{2}\sum_{k \in outputs}\left(t_{k,d} - o_{k,d}\right)^2$$

Training
Output Units

- Adjust wt $w_{ji,d}$ according to E_d as before
- For output units, this is easy since contribution of $w_{ji,d}$ to E_d when j is an output unit is the same as for single neuron case*, i.e.

$$\frac{\partial E_d}{\partial w_{ji,d}} = -\left(t_{j,d} - o_{j,d}\right) o_{j,d} \left(1 - o_{j,d}\right) x_{ji,d} = -\delta_j x_{ji,d}$$

where $\delta_j = -\frac{\partial E_d}{\partial net_j}$ = error term of unit j

*This is because all other outputs are constants w.r.t. $w_{ji,d}$

Training
Hidden Units

- How can we compute the error term for hidden layers when there is no target output $\vec{t}$ for these layers?
- Instead propagate back error values from output layer toward input layers, scaling with the weights
- Scaling with the weights characterizes how much of the error term each hidden unit is "responsible for"

Training
Hidden Units (cont'd)

The impact that $w_{ji,d}$ has on E_d is only through net_j and units immediately "downstream" of j:

$$\frac{\partial E_d}{\partial w_{ji,d}} = \frac{\partial E_d}{\partial net_j}\frac{\partial net_j}{\partial w_{ji,d}} = x_{ji}\sum_{k \in down(j)} \frac{\partial E_d}{\partial net_k}\frac{\partial net_k}{\partial net_j}$$

$$= x_{ji}\sum_{k \in down(j)} -\delta_k \frac{\partial net_k}{\partial net_j} = x_{ji}\sum_{k \in down(j)} -\delta_k \frac{\partial net_k}{\partial o_j}\frac{\partial o_j}{\partial net_j}$$

$$= x_{ji}\sum_{k \in down(j)} -\delta_k w_{kj}\frac{\partial o_j}{\partial net_j} = x_{ji}\sum_{k \in down(j)} -\delta_k w_{kj} o_j \left(1 - o_j\right)$$

Works for arbitrary number of hidden layers

Backpropagation Algorithm

Initialize all weights to small random numbers.

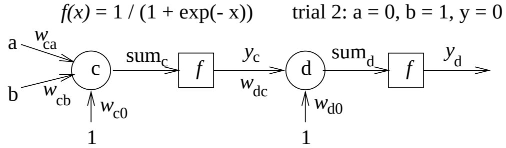
Until termination condition satisfied, Do

- For each training example, Do
  1. Input the training example to the network and compute the network outputs
  2. For each output unit k
  $$\delta_k \leftarrow o_k(1 - o_k)(t_k - o_k)$$
  3. For each hidden unit h
  $$\delta_h \leftarrow o_h(1 - o_h)\sum_{k \in down(h)} w_{k,h}\delta_k$$
  4. Update each network weight $w_{j,i}$
  $$w_{j,i} \leftarrow w_{j,i} + \Delta w_{j,i}$$
  where
  $$\Delta w_{j,i} = \eta\,\delta_j x_{j,i}$$

The Backpropagation Algorithm
Example

target = y trial 1: a = 1, b = 0, y = 1

$f(x) = 1 / (1 + \exp(-x))$ trial 2: a = 0, b = 1, y = 0

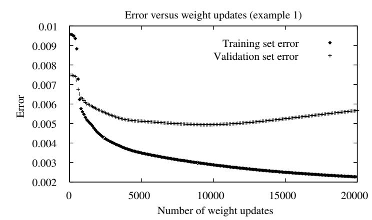


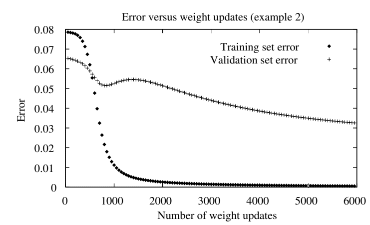
eta	0.3		
	trial 1	trial 2	
w_ca	0.1	0.1008513	0.1008513
w_cb	0.1	0.1	0.0987985
w_c0	0.1	0.1008513	0.0996498
a	1	0	
b	0	1	
const	1	1	
sum_c	0.2	0.2008513	
y_c	0.5498340	0.5500447	
w_dc	0.1	0.1189104	0.0964548
w_d0	0.1	0.1343929	0.0935679
sum_d	0.1549834	0.1997990	
y_d	0.5386685	0.5497842	
target	1	0	
delta_d	0.1146431	-0.136083	
delta_c	0.0028376	-0.004005	
delta_d(t) = y_d(t) * (y(t) - y_d(t)) * (1 - y_d(t))			
delta_c(t) = y_c(t) * (1 - y_c(t)) * delta_d(t) * w_dc(t)			
w_dc(t+1) = w_dc(t) + eta * y_c(t) * delta_d(t)			
w_ca(t+1) = w_ca(t) + eta * a * delta_c(t)			

Remarks on Backprop

- When to stop training? When weights don't change much, error rate sufficiently low, etc. (be aware of overfitting: use validation set)
- Cannot ensure convergence to global minimum due to myriad local minima, but tends to work well in practice (can re-run with new random weights)
- Generally training very slow (thousands of iterations), use is very fast
- Setting η: Small values slow convergence, large values might overshoot minimum, can adapt it over time
- Can add momentum term $\alpha < 1$ that tends to keep the updates moving in the same direction as previous trials:
$$\Delta w_{ji,d+1} = \eta\,\delta_{j,d+1}\,x_{ji,d+1} + \alpha\,\Delta w_{ji,d}$$
Can help move through small local minima to better ones & move along flat surfaces

Overfitting





Danger of stopping too soon!

Remarks on Backprop
(cont'd)

- Alternative error function: cross entropy

$$E_d = \sum_{k \in outputs} \left(t_{k,d} \ln o_{k,d} + \left(1 - t_{k,d}\right) \ln \left(1 - o_{k,d}\right)\right)$$

"blows up" if $t_{k,d} \approx 1$ and $o_{k,d} \approx 0$ or vice-versa (vs. squared error, which is always in $[0, 1]$)

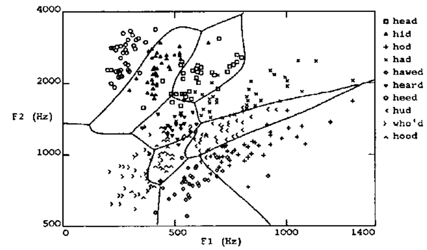
- Can penalize large weights to make space more linear and reduce risk of overfitting:

$$E_d = \frac{1}{2} \sum_{k \in outputs} (t_{kd} - o_{ok})^2 + \gamma \sum_{i,j} w_{ji,d}^2$$

- Representational power: Any boolean func. can be represented with 2 layers, any bounded, continuous func. can be rep. with arbitrarily small error with 2 layers, any func. can be rep. with arbitrarily small error with 3 layers
  - Number of required units may be large
  - GD/EG may not be able to find the right weights

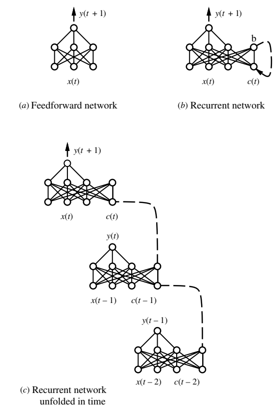
Hypothesis Space

1. Hyp. space is set of all weight vectors (continuous vs. discrete of decision trees)
2. Search via GD/EG: Possible because error function and output functions are continuous & differentiable
3. Inductive bias: (Roughly) smooth interpolation between data points



Advanced Topics

- Recurrent Networks to handle time series data (i.e. label of current ex. depends on past exs.)

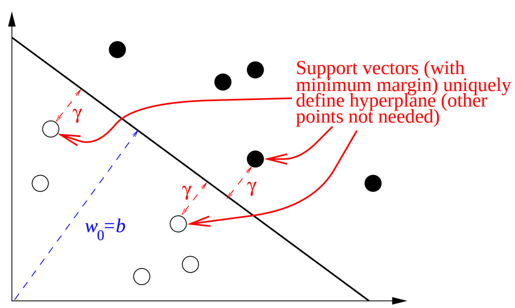


- Other optimization procedures
- Dynamically modifying network structure

Support Vector Machines
[See refs. on slides page]

- Introduced in 1992
- State-of-the-art technique for classification and regression
- Techniques can also be applied to e.g. clustering and principal components analysis
- Similar to ANNs, polynomial classifiers, and RBF networks in that it remaps inputs and then finds a hyperplane
  - Main difference is how it works
- Features of SVMs:
  - Maximization of margin
  - Duality
  - Use of kernels
  - Use of problem convexity to find classifier (often without local minima)

Support Vector Machines
Margins



- A hyperplane's margin γ is the shortest distance from it to any training vector
- Intuition: larger margin $\Rightarrow$ higher confidence in classifier's ability to generalize
  - Guaranteed generalization error bound in terms of $1/\gamma^2$ (under appropriate assumptions)
- Definition assumes linear separability (more general definitions exist that do not)

Support Vector Machines
Perceptron Algorithm Revisited

- $\vec{w}(0) \leftarrow \vec{0}$, $b(0) \leftarrow 0$, $k \leftarrow 0$, $y_i \in \{-1, +1\}\ \forall i$
- While mistakes are made on training set
  - For $i = 1$ to N (= # training vectors)
    - If $y_i\left(\vec{w}_k \cdot \vec{x}_i + b_k\right) \leq 0$
      - $\vec{w}_{k+1} \leftarrow \vec{w}_k + \eta\, y_i\, \vec{x}_i$
      - $b_{k+1} \leftarrow b_k + \eta\, y_i$
      - $k \leftarrow k + 1$
- Final predictor: $h(\vec{x}) = \mathrm{sgn}\left(\vec{w}_k \cdot \vec{x} + b_k\right)$

Support Vector Machines
Duality

- Another way of representing predictor:

$$h(\vec{x}) = \text{sgn}\,(\vec{w}\cdot\vec{x}+b) = \text{sgn}\left(\eta \sum_{i=1}^{N}(\alpha_i\, y_i\, \vec{x}_i)\cdot\vec{x}+b\right)$$
$$= \text{sgn}\left(\eta \sum_{i=1}^{N}\alpha_i\, y_i\,(\vec{x}_i\cdot\vec{x})+b\right)$$

($\alpha_i = \#$ mistakes on $\vec{x}_i$)

- So perceptron alg has equivalent dual form:
  - $\vec{\alpha} \leftarrow \vec{0}, b \leftarrow 0,$
  - While mistakes are made in For loop
    - For $i = 1$ to N ($= \#$ training vectors)
      - If $y_i\left(\eta \sum_{j=1}^{N}\alpha_j\, y_j\,\left(\vec{x}_j\cdot\vec{x}_i\right)+b\right)\le 0$

$$\alpha_i \leftarrow \alpha_i + 1$$
$$b \leftarrow b + \eta\, y_i$$

- Now data only in dot products

Kernels

- Duality lets us remap to many more features!
- Let $\vec{\phi} : \Re^\ell \rightarrow F$ be nonlinear map of f.v.s, so

$$h(\vec{x}) = \text{sgn}\left(\sum_{i=1}^{N}\alpha_i\, y_i\,\left(\vec{\phi}(\vec{x}_i)\cdot\vec{\phi}(\vec{x})\right)+b\right)$$

- Can we compute $\left(\vec{\phi}(\vec{x}_i)\cdot\vec{\phi}(\vec{x})\right)$ without evaluating $\vec{\phi}(\vec{x}_i)$ and $\vec{\phi}(\vec{x})$? YES!
- $\vec{x} = [x_1, x_2]$, $\vec{z} = [z_1, z_2]$:

$$\begin{aligned}(\vec{x}\cdot\vec{z})^2 &= (x_1 z_1 + x_2 z_2)^2\\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2\,x_1 x_2 z_1 z_2\\ &= \underbrace{\left[x_1^2, x_2^2, \sqrt{2}\,x_1 x_2\right]}_{\vec{\phi}(\vec{x})}\cdot\left[z_1^2, z_2^2, \sqrt{2}\,z_1 z_2\right]\end{aligned}$$

- LHS requires 2 mults + 1 squaring to compute, RHS takes 3 mults
- In general, $(\vec{x}\cdot\vec{z})^d$ takes ℓ mults + 1 expon., vs. $\binom{\ell+d-1}{d} \ge \left(\frac{\ell+d-1}{d}\right)^d$ mults if compute $\vec{\phi}$ first

Kernels
(cont'd)

- In general, a kernel is a function k such that $\forall\,\vec{x},\vec{z}$, $k(\vec{x},\vec{z}) = \vec{\phi}(\vec{x})\cdot\vec{\phi}(\vec{z})$
- Typically start with kernel and take the feature mapping that it yields
- E.g. Let $\ell = 1, \vec{x} = x, \vec{z} = z, k(x,z) = \sin(x-z)$
- By Fourier expansion,

$$\sin(x-z) = a_0 + \sum_{n=1}^{\infty} a_n \sin(n\,x)\sin(n\,z) + \sum_{n=1}^{\infty} a_n \cos(n\,x)\cos(n\,z)$$

for Fourier coeficients $a_0, a_1, \ldots$

- This is the dot product of two infinite sequences of nonlinear functions:

$$\{\phi_i(x)\}_{i=0}^{\infty} = [1, \sin(x), \cos(x), \sin(2x), \cos(2x), \ldots]$$

- I.e. there are an infinite number of features in this remapped space!

Kernels
(cont'd)

- Commonly-used kernels:
  - Polynomial:

$$K_{poly}(x,x') = (x\cdot x' + c)^d$$

  - Gaussian Radial Basis Function (RBF):

$$K_{RBF}(x,x') = \exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right)$$

  - Hyperbolic tangent (sigmoid):

$$K_{sig}(x,x') = \tanh(\kappa(x\cdot x') + \theta)$$

- Also have ones for structured data: e.g. graphs, trees, sequences, and sets of points

Support Vector Machines
Finding a Hyperplane

- Can show [Cristianini & Shawe-Taylor] that if data linearly separable in remapped space, then get maximum margin classifier by minimizing $\vec{w}\cdot\vec{w}$ subject to $y_i(\vec{w}\cdot\vec{x}_i + b) \ge 1$
- Can reformulate this in dual form as a convex quadratic program that can be solved optimally, i.e. won't encounter local optima:

$$\begin{aligned}\underset{\boldsymbol{\alpha}}{\text{maximize}} \quad & \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i,j}\alpha_i\,\alpha_j\,y_i\,y_j\,k(\vec{x}_i,\vec{x}_j)\\ \text{s.t.} \quad & \alpha_i \ge 0, i = 1,\ldots,m\\ & \sum_{i=1}^{m}\alpha_i\,y_i = 0\end{aligned}$$

- After optimization, we can label new vectors with the decision function:

$$f(\vec{x}) = \text{sgn}\left(\sum_{i=1}^{m}\alpha_i\,y_i\,k(\vec{x},\vec{x}_i) + b\right)$$

- Can always find a kernel that will make training set linearly separable, but beware of choosing a kernel that is too powerful (overfitting)

Support Vector Machines
Finding a Hyperplane (cont'd)

- If kernel doesn't separate, can soften the margin with slack variables ξ_i:

$$\begin{aligned}\underset{\vec{w},b,\boldsymbol{\xi}}{\text{minimize}} \quad & \|\vec{w}\|^2 + C\sum_{i=1}^{m}\xi_i\\ \text{s.t.} \quad & y_i((\vec{x}_i\cdot\vec{w}) + b) \ge 1 - \xi_i,\ i = 1,\ldots,m\\ & \xi_i \ge 0,\ i = 1,\ldots,m\end{aligned}$$

- The dual is similar to that for hard margin:

$$\begin{aligned}\underset{\boldsymbol{\alpha}}{\text{maximize}} \quad & \sum_{i=1}^{m}\alpha_i - \sum_{i,j}\alpha_i\,\alpha_j\,y_i\,y_j\,k(x_i,x_j)\\ \text{s.t.} \quad & 0 \le \alpha_i \le C,\ i = 1,\ldots,m\\ & \sum_{i=1}^{m}\alpha_i\,y_i = 0\end{aligned}$$

- Can still solve optimally
- If number of training vectors is very large, may opt to approximately solve these problems to save time and space
- Use e.g. gradient ascent and sequential minimal optimization (SMO) [Cristianini & Shawe-Taylor]
- When done, can throw out non-SVs

Topic summary due in 1 week!