Lecture 26: Neural Nets

ECE 417: Multimedia Signal Processing
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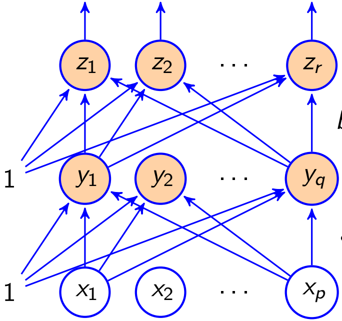
University of Illinois

11/30/2017

Outline

Two-Layer Feedforward Neural Network



$$\vec{z} = h(\vec{x}, U, V)$$

$$z_\ell = g(b_\ell) \qquad \vec{z} = g(\vec{b})$$

$$b_\ell = v_{k0} + \sum_{k=1}^{q} v_{\ell k} y_k \qquad \vec{b} = V\vec{y}$$

$$y_k = f(a_k) \qquad \vec{y} = f(\vec{a})$$

$$a_k = u_{k0} + \sum_{j=1}^{p} u_{kj} x_j \qquad \vec{a} = U\vec{x}$$

$\vec{x}$ is the input vector

Neural Network = Universal Approximator

Assume. . .

- Linear Output Nodes: $g(b) = b$
- Smoothly Nonlinear Hidden Nodes: $f'(a) = \frac{df}{da}$ finite
- Smooth Target Function: $\vec{z} = h(\vec{x}, U, V)$ approximates $\vec{\zeta} = h^*(\vec{x}) \in \mathcal{H}$, where $\mathcal{H}$ is some class of sufficiently smooth functions of $\vec{x}$ (functions whose Fourier transform has a first moment less than some finite number C)
- There are q hidden nodes, y_k, $1 \leq k \leq q$
- The input vectors are distributed with some probability density function, $p(\vec{x})$, over which we can compute expected values.

Then (Barron, 1993) showed that. . .

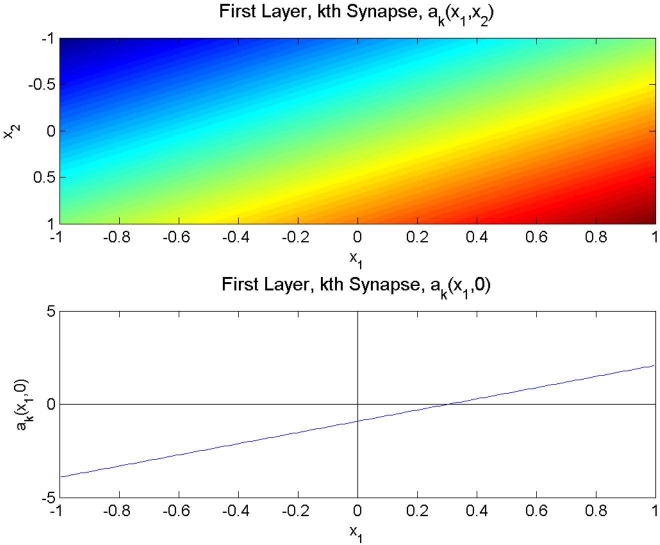
$$\max_{h^*(\vec{x})\in\mathcal{H}} \min_{U,V} E\left[h(\vec{x}, U, V) - h^*(\vec{x})|^2\right] \leq \mathcal{O}\left\{\frac{1}{q}\right\}$$

Neural Network Problems: Outline of Remainder of this Talk

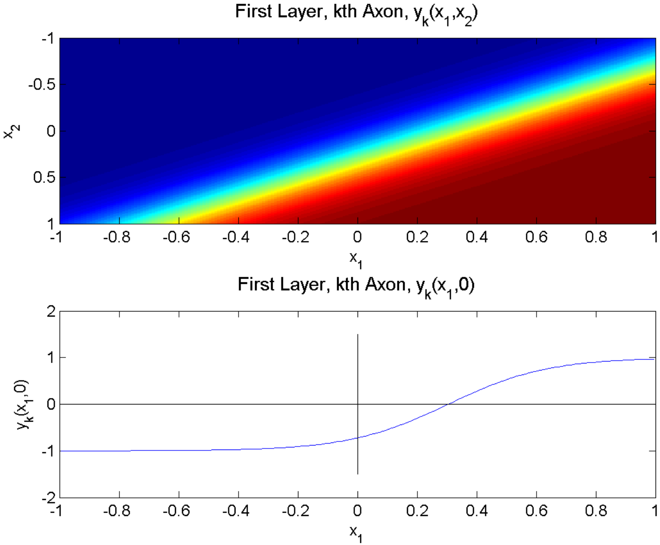
1. **Knowledge-Based Design.** Given U, V, f, g, what kind of function is $h(\vec{x}, U, V)$? Can we draw $\vec{z}$ as a function of $\vec{x}$? Can we heuristically choose U and V so that $\vec{z}$ looks kinda like $\vec{\zeta}$?
2. **Error Metric.** In what way should $\vec{z} = h(\vec{x})$ be "similar to" $\vec{\zeta} = h^*(\vec{x})$?
3. **Local Optimization: Gradient Descent with Back-Propagation.** Given an initial U, V, how do I find $\hat{U}$, $\hat{V}$ that more closely approximate $\vec{\zeta}$?
4. **Global Optimization: Simulated Annealing.** How do I find the globally optimum values of U and V?

Outline

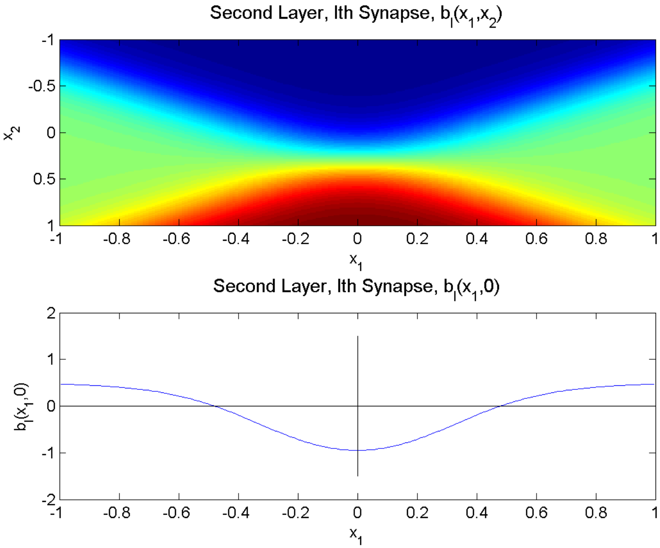
Synapse, First Layer: $a_k = u_{k0} + \sum_{j=1}^{2} u_{kj} x_j$



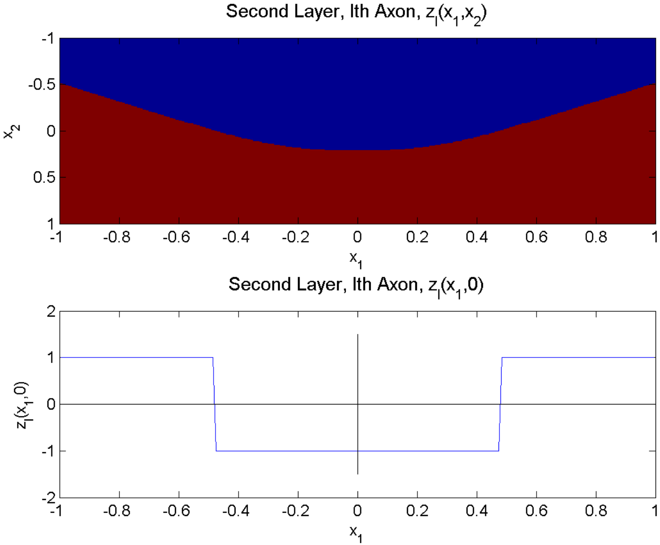
Axon, First Layer: $y_k = \tanh(a_k)$



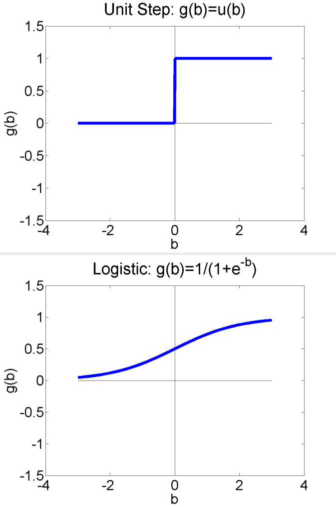
Synapse, Second Layer: $b_\ell = v_{\ell 0} + \sum_{k=1}^{2} v_{\ell k} y_k$



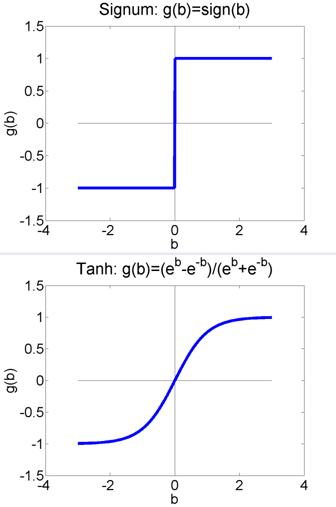
Axon, Second Layer: $z_\ell = \text{sign}(b_\ell)$



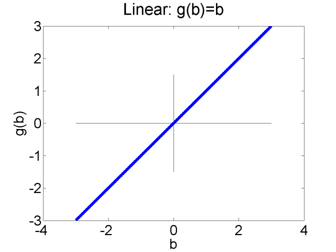
Step and Logistic nonlinearities

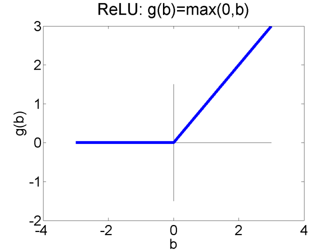


Signum and Tanh nonlinearities



"Linear Nonlinearity" and ReLU





Max and Softmax

Max:

$$z_\ell = \begin{cases} 1 & b_\ell = \max_m b_m \\ 0 & \text{otherwise} \end{cases}$$

Softmax:

$$z_\ell = \frac{e^{b_\ell}}{\sum_m e^{b_m}}$$

Outline

Error Metric: How should $h(\vec{x})$ be "similar to" $h^*(\vec{x})$?

Linear output nodes:

Minimum Mean Squared Error (MMSE)

$$U^*, V^* = \arg\min E_n = \arg\min \frac{1}{n}\sum_{i=1}^{n} |\vec{\zeta}_i - \vec{z}(x_i)|^2$$

MMSE Solution: $\vec{z} = E\left[\vec{\zeta}|\vec{x}\right]$

If the training samples $(\vec{x}_i, \vec{\zeta}_i)$ are i.i.d., then

$$E_\infty = E\left[|\vec{\zeta} - \vec{z}|^2\right]$$

E_∞ is minimized by

$$\vec{z}_{MMSE}(\vec{x}) = E\left[\vec{\zeta}|\vec{x}\right]$$

Error Metric: How should $h(\vec{x})$ be "similar to" $h^*(\vec{x})$? Logistic output nodes:

Binary target vector

Suppose

$$\zeta_\ell = \begin{cases} 1 & \text{with probability } P_\ell(\vec{x}) \\ 0 & \text{with probability } 1 - P_\ell(\vec{x}) \end{cases}$$

and suppose $0 \leq z_\ell \leq 1$, e.g., logistic output nodes.

MMSE Solution: $z_\ell = \Pr\{\zeta_\ell = 1|\vec{x}\}$

$$\begin{aligned} E[\zeta_\ell|\vec{x}] &= 1 \cdot P_\ell(\vec{x}) + 0 \cdot (1 - P_\ell(\vec{x})) \\ &= P_\ell(\vec{x}) \end{aligned}$$

So the MMSE neural network solution is

$$z_{\ell,MMSE}(\vec{x}) = P_\ell(\vec{x})$$

Error Metric: How should $h(\vec{x})$ be "similar to" $h^*(\vec{x})$? Softmax output nodes:

One-Hot Vector, MKLD Solution: $z_\ell = \Pr\{\zeta_\ell = 1|\vec{x}\}$

- Suppose $\vec{\zeta}_i$ is a "one hot" vector, i.e., only one element is "hot" ($\zeta_{\ell(i),i} = 1$), all others are "cold" ($\zeta_{mi} = 0$, $m \neq \ell(i)$).
- MMSE will approach the solution $z_\ell = \Pr\{\zeta_\ell = 1|\vec{x}\}$, but there's no guarantee that it's a correctly normalized pmf ($\sum z_\ell = 1$) until it has fully converged.
- MKLD also approaches $z_\ell = \Pr\{\zeta_\ell = 1|\vec{x}\}$, and guarantees that $\sum z_\ell = 1$. MKLD is also more computationally efficient, if $\vec{\zeta}$ is a one-hot vector.

MKLD = Minimum Kullback-Leibler Distortion

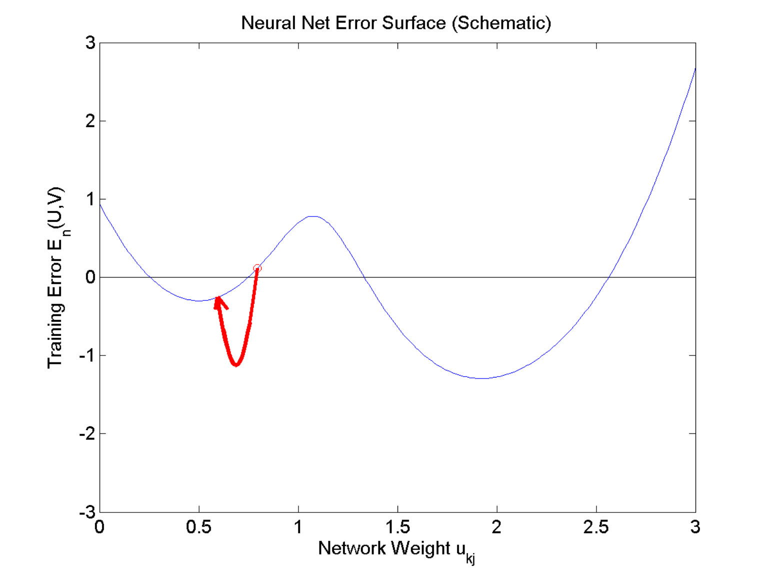
$$D_n = \frac{1}{n}\sum_{i=1}^{n}\sum_{\ell=1}^{r}\zeta_{\ell i}\log\left(\frac{\zeta_{\ell i}}{z_{\ell i}}\right) = -\frac{1}{n}\sum_{i=1}^{n}\log z_{\ell(i),i}$$

Error Metrics Summarized

- Use MSE to achieve $\vec{z} = E\left[\vec{\zeta}|\vec{x}\right]$. That's almost always what you want.
- If $\vec{\zeta}$ is a one-hot vector, then use KLD (with a softmax nonlinearity on the output nodes) to guarantee that $\vec{z}$ is a properly normalized probability mass function, and for better computational efficiency.
- If ζ_ℓ is binary, but not necessarily one-hot, then use MSE (with a logistic nonlinearity) to achieve $z_\ell = \Pr\left\{\zeta_\ell = 1|\vec{x}\right\}$.
- If ζ_ℓ is signed binary ($\zeta_\ell \in \{-1, +1\}$, then use MSE (with a tanh nonlinearity) to achieve $z_\ell = E\left[\zeta_\ell|\vec{x}\right]$.
- After you're done training, you can make your cell phone app more efficient by throwing away the uncertainty:
  - Replace softmax output nodes with max
  - Replace logistic output nodes with unit-step
  - Replace tanh output nodes with signum

Outline

Gradient Descent = Local Optimization



Gradient Descent = Local Optimization

Given an initial U, V, find $\hat{U}$, $\hat{V}$ with lower error.

$$
\begin{aligned}
\hat{u}_{kj} &= u_{kj} - \eta \frac{\partial E_n}{\partial u_{kj}} \\
\hat{v}_{\ell k} &= v_{\ell k} - \eta \frac{\partial E_n}{\partial v_{\ell k}}
\end{aligned}
$$

η =Learning Rate

- If η too large, gradient descent won't converge. If too small, convergence is slow. Usually we pick $\eta \approx 0.001$ and cross our fingers.
- Second-order methods like L-BFGS choose an optimal η at each step, so they're MUCH faster.

Computing the Gradient

OK, let's compute the gradient of E_n with respect to the V matrix. Remember that V enters the neural net computation as $b_{\ell i} = \sum_k v_{\ell k} y_{ki}$, and then z depends on b somehow. So...

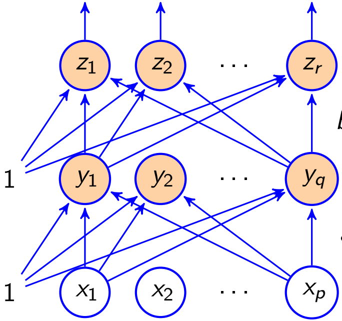
$$\begin{aligned} \frac{\partial E_n}{\partial v_{\ell k}} &= \sum_{i=1}^{n} \left(\frac{\partial E_n}{\partial b_{\ell i}} \right) \left(\frac{\partial b_{\ell i}}{\partial v_{\ell k}} \right) \\ &= \sum_{i=1}^{n} \epsilon_{\ell i} y_{ki} \end{aligned}$$

where the last line only works if we define $\epsilon_{\ell i}$ in a useful way:

Back-Propagated Error

$$\epsilon_{\ell i} = \frac{\partial E_n}{\partial b_{\ell i}} = \frac{2}{n}(z_{\ell i} - \zeta_{\ell i}) g'(b_{\ell i})$$

where $g'(b) = \frac{\partial g}{\partial b}$.



$$\vec{z} = h(\vec{x}, U, V)$$

$$z_\ell = g(b_\ell) \qquad \vec{z} = g(\vec{b})$$

$$b_\ell = v_{k0} + \textstyle\sum_{k=1}^{q} v_{\ell k} y_k \qquad \vec{b} = V\vec{y}$$

$$y_k = f(a_k) \qquad \vec{y} = f(\vec{a})$$

$$a_k = u_{k0} + \textstyle\sum_{j=1}^{p} u_{kj} x_j \qquad \vec{a} = U\vec{x}$$

$\vec{x}$ is the input vector

Back-Propagating to the First Layer

$$\frac{\partial E_n}{\partial u_{kj}} = \sum_{i=1}^{n} \left(\frac{\partial E_n}{\partial a_{ki}}\right)\left(\frac{\partial a_{ki}}{\partial u_{kj}}\right) = \sum_{i=1}^{n} \delta_{ki} x_{ji}$$

where... $\delta_{ki} = \dfrac{\partial E_n}{\partial a_{ki}} = \displaystyle\sum_{\ell=1}^{r} \epsilon_{\ell i} v_{\ell k} f'(a_{ki})$

The Back-Propagation Algorithm

$$\hat{V} = V - \eta \nabla_V E_n, \qquad \hat{U} = U - \eta \nabla_U E_n$$

$$\nabla_V E_n = E Y^T, \qquad \nabla_U E_n = D X^T$$

$$Y = [\vec{y}_1, \ldots, \vec{y}_n], \qquad X = [\vec{x}_1, \ldots, \vec{x}_n]$$

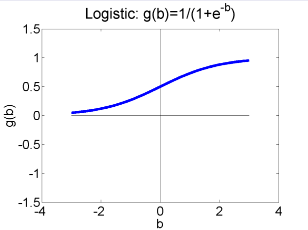
$$E = [\vec{\epsilon}_1, \ldots, \vec{\epsilon}_n], \qquad D = \left[\vec{\delta}_1, \ldots, \vec{\delta}_n\right]$$

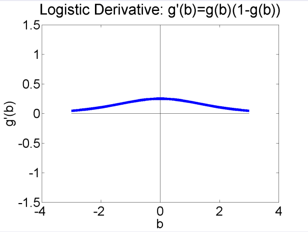
$$\vec{\epsilon}_i = \frac{2}{n} g'(\vec{b}_i) \odot \left(\vec{z}_i - \vec{\zeta}_i\right), \qquad \vec{\delta}_i = f'(\vec{a}_i) \odot V^T \vec{\epsilon}_i$$

... where $\odot$ means element-wise multiplication of two vectors; $g'(\vec{b})$ and $f'(\vec{a})$ are element-wise derivatives of the $g(\cdot)$ and $f(\cdot)$ nonlinearities.

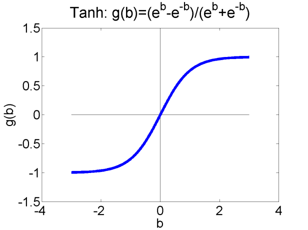
Derivatives of the Nonlinearities

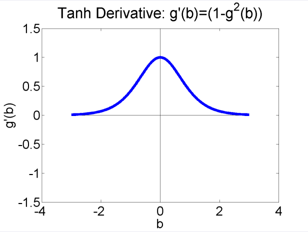
Logistic



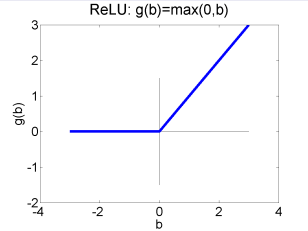


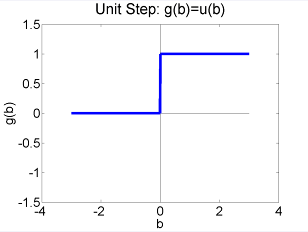
Tanh





ReLU





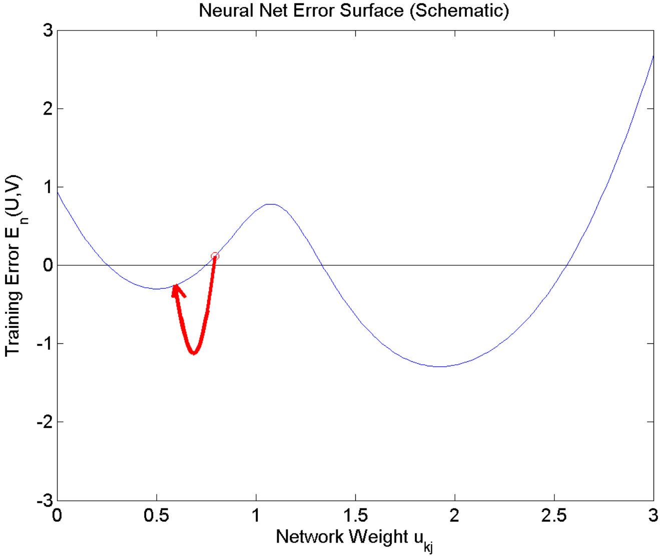
Outline

Simulated Annealing: How can we find the globally optimum U, V?

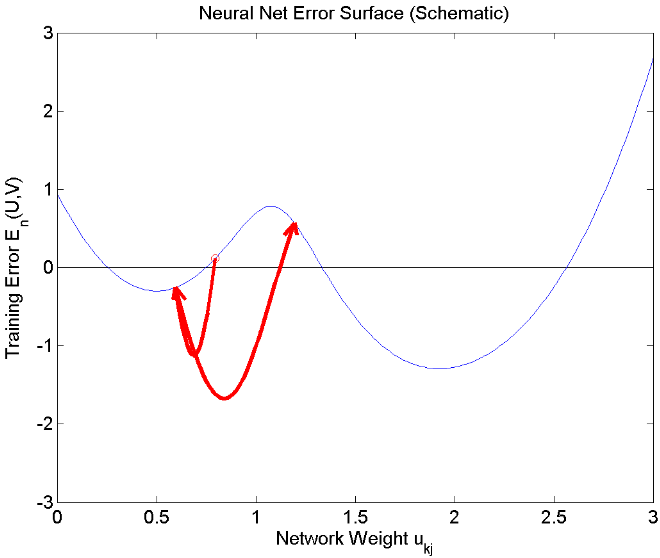
- Gradient descent finds a local optimum. The $\hat{U}, \hat{V}$ you end up with depends on the U, V you started with.
- How can you find the **global optimum** of a non-convex error function?
- The answer: Add randomness to the search, in such a way that...

$$P(\text{reach global optimum}) \xrightarrow{t\rightarrow\infty} 1$$

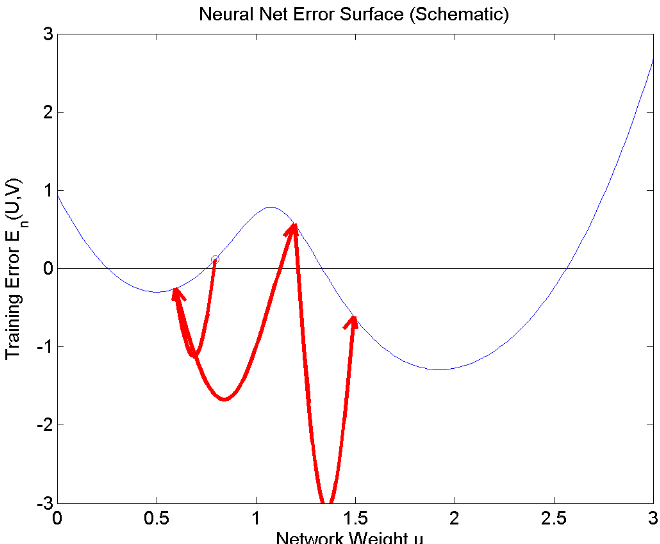
- Take a random step. If it goes downhill, do it.



- Take a random step. If it goes downhill, do it.
- If it goes uphill, SOMETIMES do it.



- Take a random step. If it goes downhill, do it.
- If it goes uphill, SOMETIMES do it.
- Uphill steps become less probable as $t \to \infty$



Simulated Annealing: Algorithm

FOR $t = 1$ TO ∞, DO

1. Set $\hat{U} = U + \text{RANDOM}$
2. If your random step caused the error to decrease ($E_n(\hat{U}) < E_n(U)$), then set $U = \hat{U}$ (**prefer to go downhill**)
3. Else set $U = \hat{U}$ with probability P (**. . . but sometimes go uphill!**)
   1. $P = \exp(-(E_n(\hat{U}) - E_n(U))/\text{Temperature})$ (**Small steps uphill are more probable than big steps uphill.**)
   2. $\text{Temperature} = T_{max}/\log(t+1)$ (**Uphill steps become less probable as $t \to \infty$.**)
4. Whenever you reach a local optimum (U is better than both the preceding and following time steps), check to see if it's better than all preceding local optima; if so, remember it.

Convergence Properties of Simulated Annealing

(Hajek, 1985) proved that, if we start out in a "valley" that is separated from the global optimum by a "ridge" of height T_{max}, and if the temperature at time t is $T(t)$, then simulated annealing converges in probability to the global optimum if

$$\sum_{t=1}^{\infty} \exp\left(-T_{max}/T(t)\right) = +\infty$$

For example, this condition is satisfied if

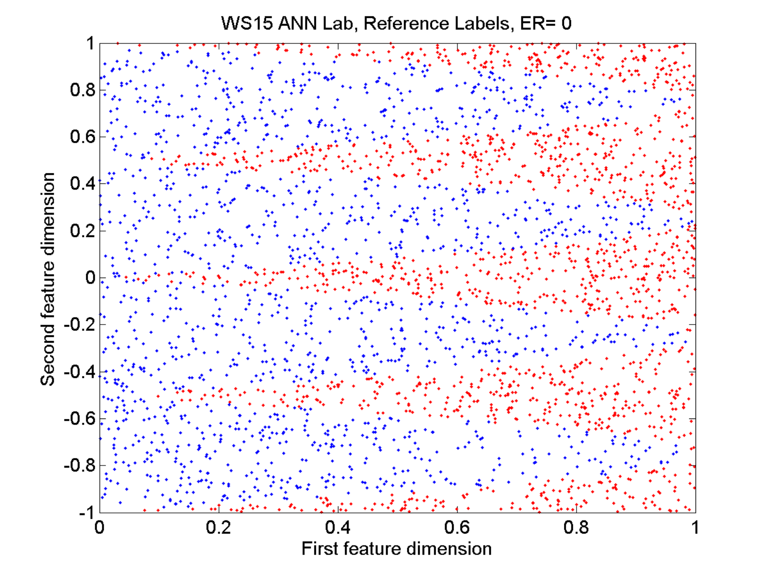
$$T(t) = T_{max}/\log(t+1)$$

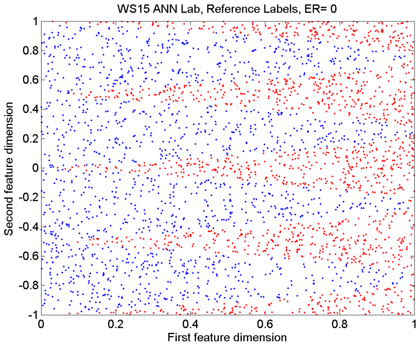
Real-World Randomness: Stochastic Gradient Descent (SGD)

- SGD is the following algorithm. For `t=1:T`,
  1. Randomly choose a small subset of your training data (a **minibatch**: strictly speaking, SGD is minibatch size of $m = 1$, but practical minibatches are typically $m \sim 100$)
  2. Perform a complete backprop iteration using the minibatch.
- Advantage of SGD over Simulated Annealing: computational complexity
  - Instead of introducing randomness with a random weight update ($\mathcal{O}\left\{n\right\}$), we introduce randomness by randomly sampling the dataset ($\mathcal{O}\left\{m\right\}$)
  - Matters a lot when n is large
- Disadvantage of SGD over Simulated Annealing: It's not theoretically proven to converge to a global optimum
  - ... but it works in practice, if training dataset is big enough.

Outline

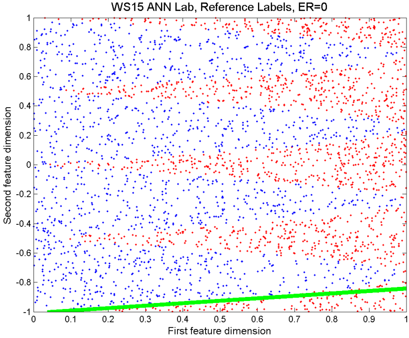
Here's the dataset





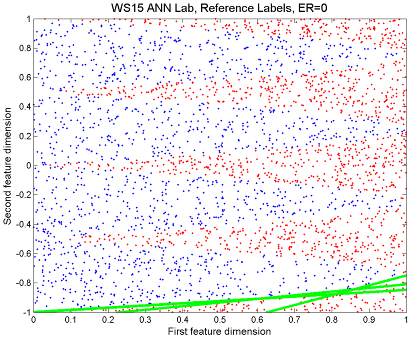
Knowledge-based design: set each row of U to be a line segment, $u_0 + u_1 x_1 + u_2 x_2 = 0$, on the decision boundary.
u_0 is an arbitrary scale factor; $u_0 = -20$ makes the tanh work well.

```
[x1,x2]=ginput(2);
u0=-20;   % Arbitrary scale factor
u = -inv([x1,x2])*[u0;u0];
U(1,:) = [u0,u(1),u(2)];
```



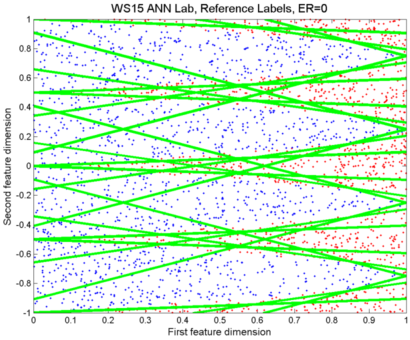
Check your math by plotting $x_2 = -\frac{u_0}{u_2} - \frac{u_1}{u_2}x_1$

```
nnplot(X,ZETA,ZETA,'Reference Labels',1);
hold on;
plot([0,1],-(u0/u(2))+[0,-u(1)/u(2)],'g-');
hold off;
```



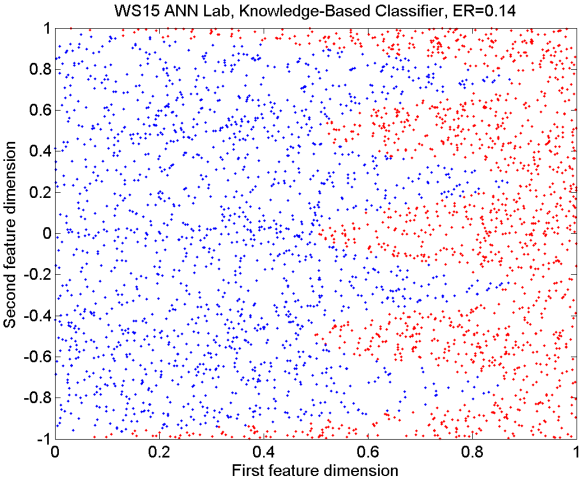
Here are 3 such segments, mapping out the lowest curve:

```
for m=1:3,
plot([0 1],-U(m,1)/U(m,3)+[0,-U(m,2)/U(m,3)]);
end
```



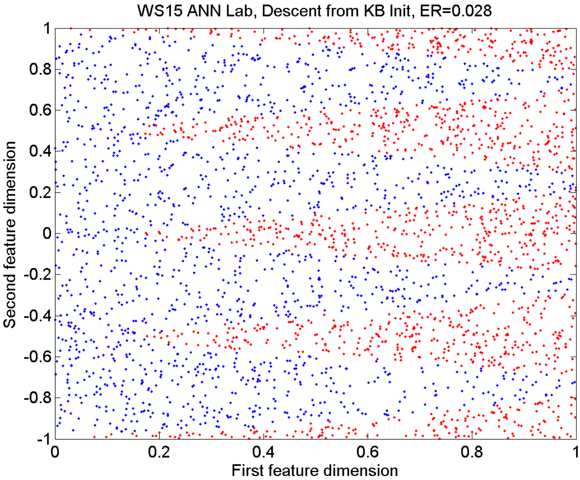
(1) Reflect through $x_2 = -0.75$, and (2) Shift upward:

```
Ufoo = [U; U(:,1)-1.5*U(:,3),U(:,2),-U(:,3)];
Ubar = [Ufoo; Ufoo-[0.5*Ufoo(:,3),zeros(6,2)]];
U =  [Ubar; Ubar-[Ubar(:,3),zeros(12,2)]];
```



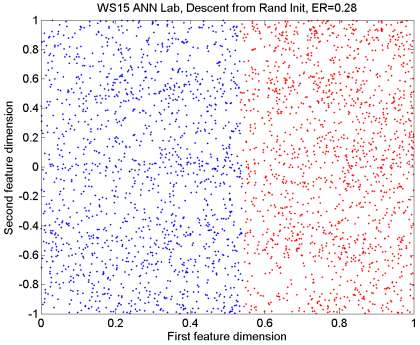
nnclassify.m: Error Rate = 14%

```
function [Z,Y]=nnclassify(X,U,V)
Y = tanh(U*[ones(1,n); X]);
Z = tanh(V*[ones(1,n); Y]);
```



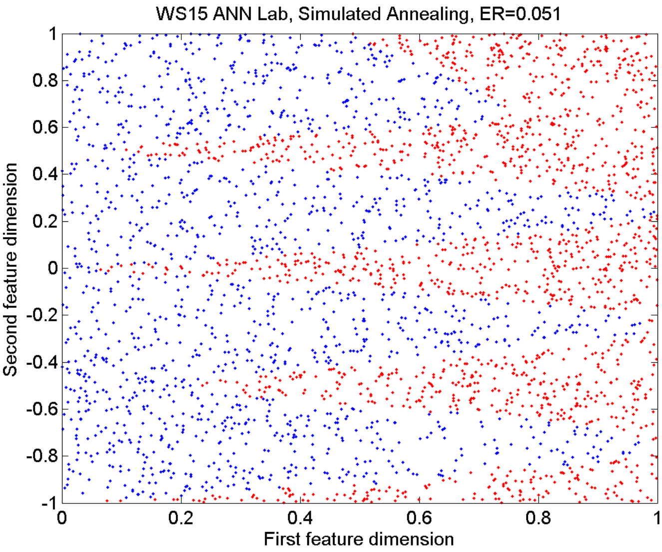
nnbackprop.m: Error Rate = 2.8%

```
function [EPSILON,DELTA]=nnbackprop(X,Y,Z,ZETA,V)
EPSILON = 2* (1-Z.^2) .* (Z-ZETA);
DELTA = (1-Y.^2) .* (V(:,2:(q+1))' * EPSILON);
```



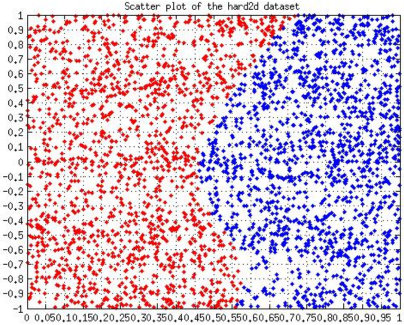
But with random initialization: Error Rate = 28%

```
Urand = [0.02*randn(q,p+1)];
Vrand = [0.02*randn(r,q+1)];
[Uc,Vc] = nndescent(X,ZETA,Urand,Vrand,0.1,1000);
[Zc,Yc] = nnclassify(X,Uc,Vc);
```


WS15 ANN Lab, Simulated Annealing, ER=0.051
Second feature dimension
First feature dimension
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
0.2
0.4
0.6
0.8
1

nnanneal.m: Error Rate $= 5.1\%$

```
function [Es,Us,Vs] = nnanneal(X,ZETA,U0,V0,ETA,T)
for t=1:T,
 U1=U0+randn(q,p+1); V1=V0+randn(r,q+1);
 ER1 = sum(nnclassify(X,U1,V1).*ZETA<0)/n;
 if ER1 < ER0,
   U0=U1;V0=V1;ER0=ER1;
 else
   P = exp(-(ER1-ER0)*log(t+1)/ridge);
   if rand() < P,
    U0=U1;V0=V1;ER0=ER1;
```

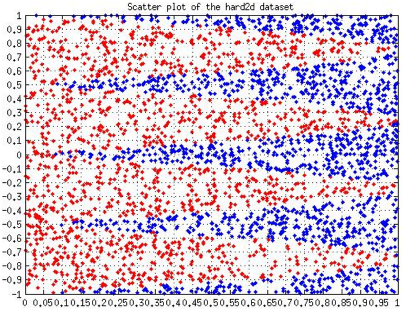


Here's one that Amit tried based on my mistaken early draft of the instructions for this lab. Error Rate: 28%

```
temperature=ridge/sqrt(t);
```

instead of the correct form,

```
temperature=ridge/log(t+1);
```



. . . and Amit solved it using Geometric Annealing. Error Rate: 0.67%

- Smaller random steps: $\Delta U \sim \mathcal{N}(0, 1e-4)$ instead of $\mathcal{N}(0,1)$, and only one weight at a time instead of all weights at once
- Geometric annealing: temperature cools geometrically ($T(t) = \alpha T(t-1)$) rather than logarithmically $T(t) = c/\log(t+1)$

Simulated Annealing: More Results

Algorithm	c or α	t	Error Rate
Hajek Cooling	1	52356	5.1%
$(T = c/\log(t+1))$	10^{-4}	1800	0.70%
Geometric Annealing	0.7	500	0.43%
$T(t) = \alpha T(t-1)$	0.8	500	0.40%
	0.9	500	0.80%

More Comments on Simulated Annealing

- Gaussian random walk results in very large weights
  - I fought this using the `mod` operator, to map weights back to the range $[-25, 25]$
  - I suspect it matters, but I'm not sure
- Every time you reach a new low error,
  - Store it, and its associated weights, in case you never find it again, and
  - Print it on the screen (using `disp` and `sprintf`) so you can see how your code is doing
- Simulated annealing can take a really long time.

Outline

Conclusions

- Back-prop.
  - You need to know how to do it.
  - ...but back-prop is only useful if you start from a good initial set of weights, or if you have good randomness
- Knowledge-based initialization
  - Sometimes, it helps if you understand what you're doing.
- Stochastic search.
  - Simulated annealing: guaranteed performance, high complexity.
  - Stochastic gradient descent: not guaranteed, but low complexity. Incidentally, I haven't tried it yet on `hard2d.txt`; if you try it, please tell me how it works.