MACHINE LEARNING AND PATTERN RECOGNITION

Spring 2004, Lecture 02b: Energy-Based Models and Loss Functions, Linear Machines

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Linear Machines: Regression with Mean Square

Linear Regression, Mean Square Loss:

- decision rule: $y = W'X$
- loss function: $L(W, y^i, X^i) = \frac{1}{2}(y^i - W'X^i)^2$
- gradient of loss: $\frac{\partial L(W,y^i,X^i)}{\partial W}' = -(y^i - W(t)'X^i)X^i$
- update rule: $W(t+1) = W(t) + \eta(t)(y^i - W(t)'X^i)X^i$

Linear Machines: Perceptron

Perceptron:

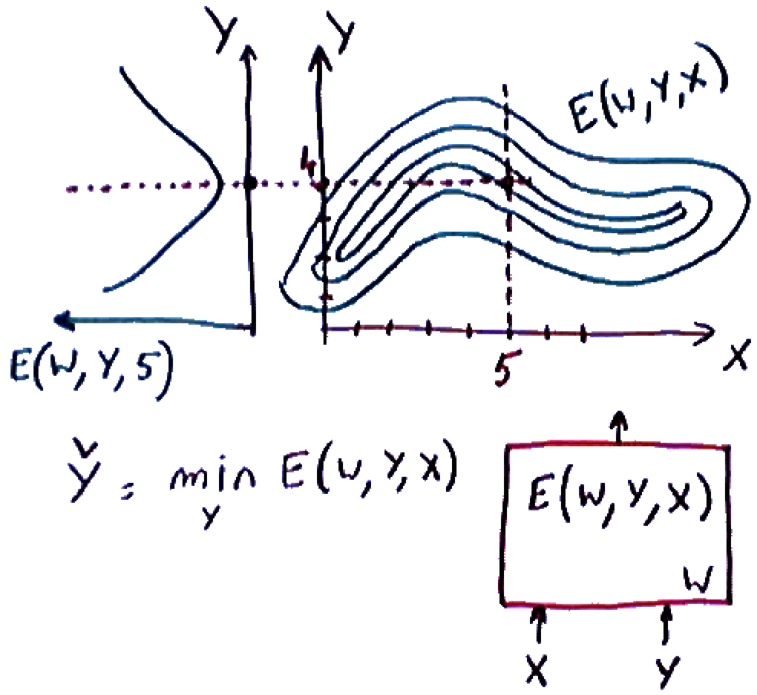
- decision rule: $y = F(W'X)$ (F is the threshold function)
- loss function: $L(W, y^i, X^i) = -(y^i - F(W'X^i))W'X$
- gradient of loss: $\frac{\partial L(W,y^i,X^i)}{\partial W}' = -(y^i - F(W(t)'X^i))X^i$
- update rule: $W(t+1) = W(t) + \eta(t)(y^i - F(W(t)'X^i))X^i$

Linear Machines: Logistic Regression

Logistic Regression, Negative Log-Likelihood Loss function:

- decision rule: $y = F(W'X)$, with $F(a) = \tanh(a)$ (sigmoid function).
- loss function: $L(W, y^i, X^i) = \log(1 + \exp(-y^i W' X^i))$
- gradient of loss: $\frac{\partial L(W, y^i, X^i)}{\partial W}' = -\left(Y^i - F(W'X)\right) X^i$
- update rule: $W(t+1) = W(t) + \eta(t)(y^i - F(W(t)'X^i))X^i$

Energy-Based Models

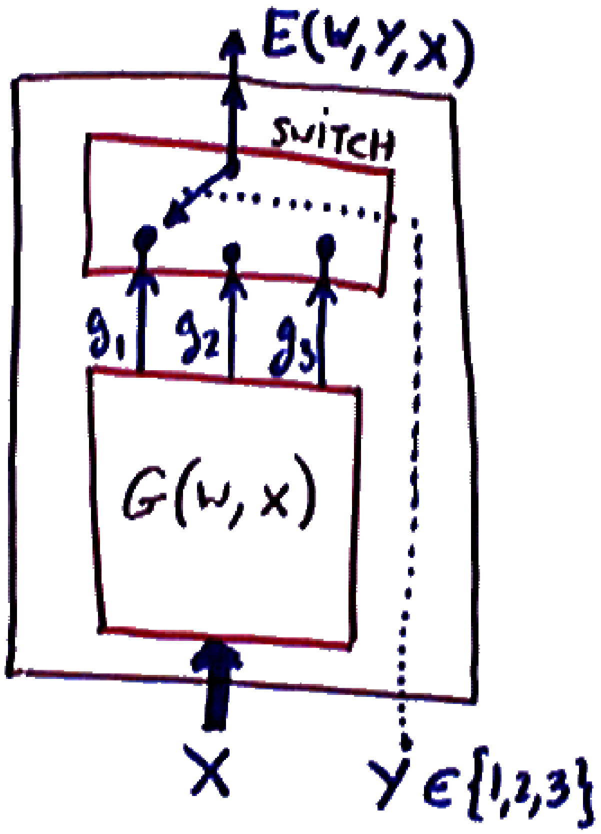


- An energy-based model is a scalar-valued *energy function*: $E(W, Y, X)$.
- X is the input, and Y the variable to be predicted (output).
- W is the parameter vector to be learned.
- X and Y can be discrete variables, scalars, vectors, tensors, sequences, probability distributions, or any other entity.

Minimum Energy Machine: Operating the machine (performing an *inference*), consists in taking an input X, and looking for the value of Y within a permissible set $\{Y\}$, that minimizes $E(W, Y, X)$:

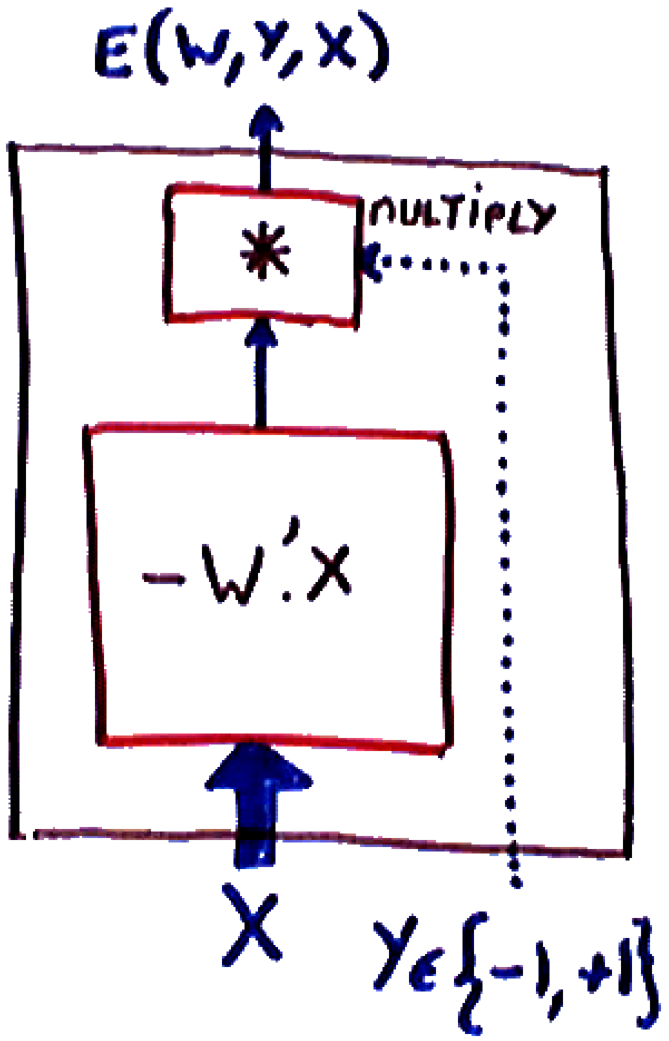
$$\check{Y} = \text{argmin}_{Y \in \{Y\}} E(W, Y, X)$$

Examples of EBM: Classifier



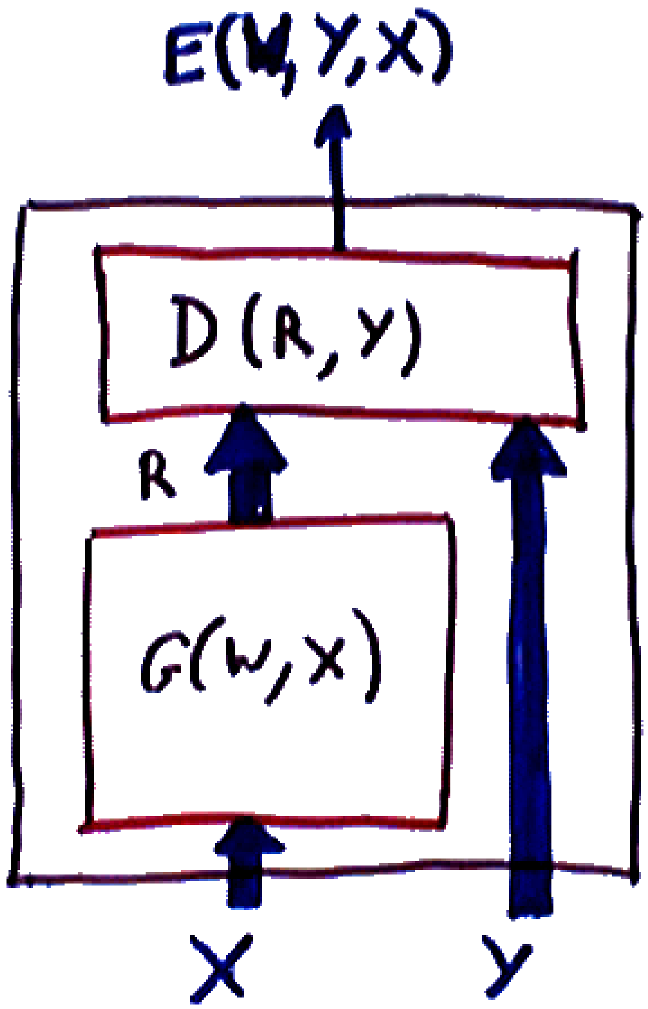
- Y is a discrete variable, $\{Y\} = \{1, 2, 3\}$.
- Energy: $E(W, Y, X) = \sum_k G_k(W, X)\delta(k, Y)$, where $\delta(k, Y) = 1$ iff $k = Y$ and 0 otherwise.
- $G_k(W, X)$, the k-th component of the output vector of $G(W, X)$ is interpreted as the "cost" of classifying X into category k.
- Best output: $\check{Y} = \min_{Y \in \{Y\}} E(W, Y, X) = \min_k G_k(W, X)$.

Examples of EBM Classifier: Perceptron



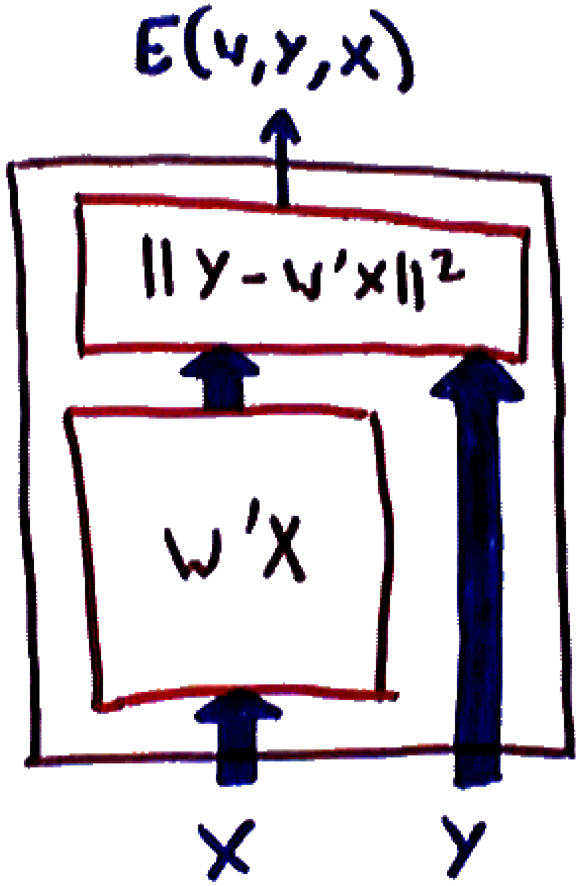
- Y is a discrete variable, $\{Y\} = \{-1, +1\}$.
- Energy: $E(W, Y, X) = -Y.W'X$.
- Best output: $\check{Y} = \text{sign}(W'X)$, where $\text{sign}(R) = +1$ iff $R > 0$ and -1 otherwise.

Examples of EBM: Regressor



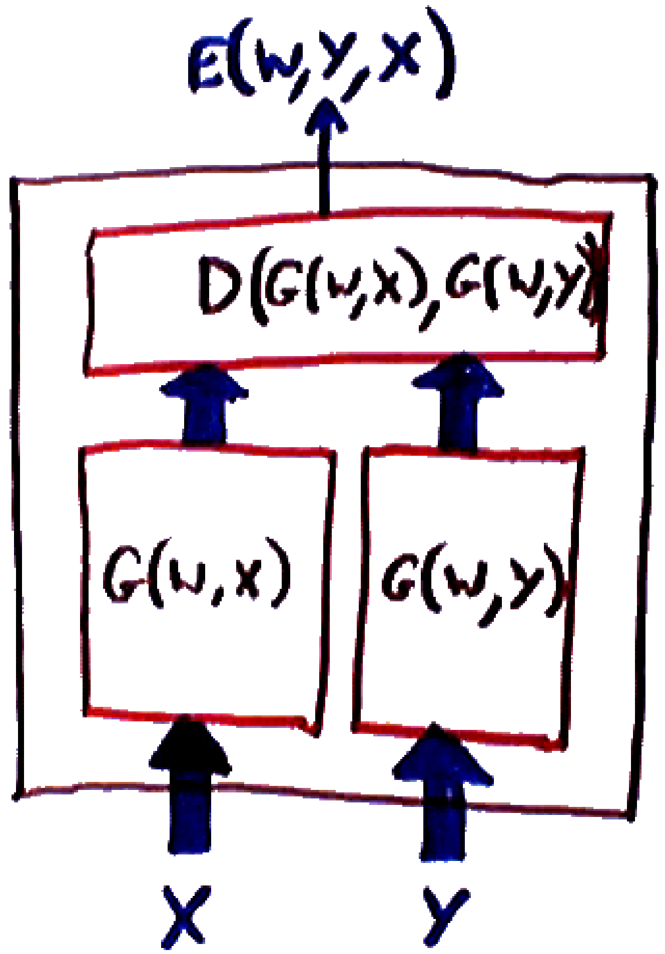
- X and Y are vectors or other entities
- Energy: $E(W,Y,X) = D(Y,G(W,X))$ where $D(Y,R)$ is a distance or dissimilarity measure.
- Best output: $\check{Y} = \min_Y E(W,Y,X) = G(W,X)$.

Examples of EBM Regressor: Linear Regression



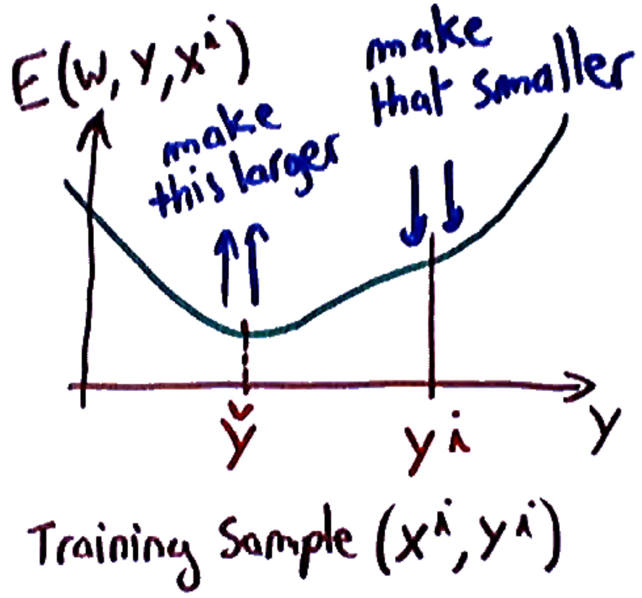
- X and Y are vectors
- Energy: $E(W,Y,X) = ||Y - W'X)||^2$.
- Best output: $\check{Y} = \min_Y E(W,Y,X) = W'X$.

Examples of EBM: Matcher



- X and Y are vectors of the same dimension.
- Energy:
  $E(W,Y,X) = D(G(W,Y),G(W,X))$ where
  $D(.,.)$ is a distance or dissimilarity measure.
- Best output: $\check{Y} = \min_Y E(W,Y,X) = G^(- 1)(G(W,X))$.

Training Energy-Based Models



- To train an EBM, we minimize a **loss function**, which is an average over training samples of a **per-sample loss function** $L(W, Y^i, X^i)$:

$$\mathcal{L}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} L(W, Y^i, X^i)$$

- The loss function must be designed so that minimizing it with respect to W will make the machine approach the desired behavior.

To ensure this, we pick loss functions that, for a given training input X^i, will drive the energies $E(W, Y^i, X^i)$ associated with the desired output Y^i to be lower than the energies associated with all other (undesired) outputs values $E(W, Y, X^i)$ for all $Y \neq Y^i, Y \in \{Y\}$.

Form of the Loss Function

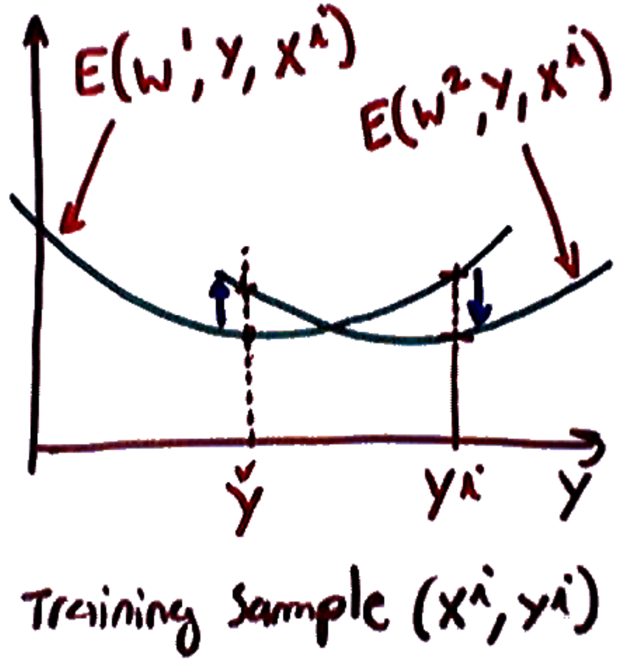
- We assume that the per-sample loss function $L(W, Y^i, X^i)$ has a lower bound over W for all Y^i, X^i.
- We assume that L depends on X^i only indirectly through the set of energies $\{E(W, Y, X^i)\ ,\ Y \in \{Y\}\}$.
- For example, if $\{Y\}$is the set of integers between 0 and $k-1$ (as would be the case for a classifier with k categories), the per-sample loss for sample (X^i, Y^i) should be of the form:

$$L(W, Y^i, X^i) = L(Y^i, E(W, 0, X^i), E(W, 1, X^i), \ldots, E(W, k-1, X^i))$$

- With this assumption, we separate the choice of the loss function from the details of the internal structure of the machine, and limit the discussion to how minimizing the loss function affects the energies.

Examples of Loss: Energy Loss

Energy Loss, the simplest of all losses: $L_{\text{energy}}(W, Y^i, X^i) = E(W, Y^i, X^i)$. This loss only works if $E(W, Y^, X^i)$ has a special form which guarantess that making $E(W, Y^i, X^i)$ lower will automatically make $E(W, Y, X^i)$ for $Y \neq Y^i$ larger than the minimum.



Training Sample (X^i, Y^i)

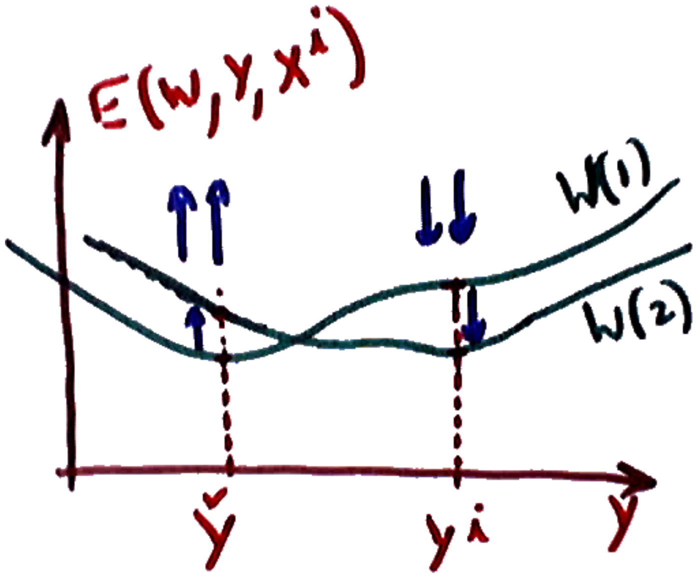
<span style="color:red">Example</span>: if $E(W, Y, X)$ is quadratic in Y, as is the case for regression with squared error: $E(W, Y, X) = ||Y - G(W, X)||^2$,
Let $W(1)$ is the parameter before a learning update, and $W(2)$ the parameter after the learning update, and let $\check{Y} = \min_Y E(W(1), Y, X)$. Then,

$$E(W(2), Y^i, X^i) - E(W(2), \check{Y}, X^i) < E(W(1), Y^i, X^i) - E(W(1), \check{Y}, X^i)$$

Examples of Loss: Perceptron Loss

Perceptron Loss:

$$L_{\text{perceptron}}(W, Y^i, X^i) = E(W, Y^i, X^i) - \min_{Y \in \{Y\}} E(W, Y, X^i)$$



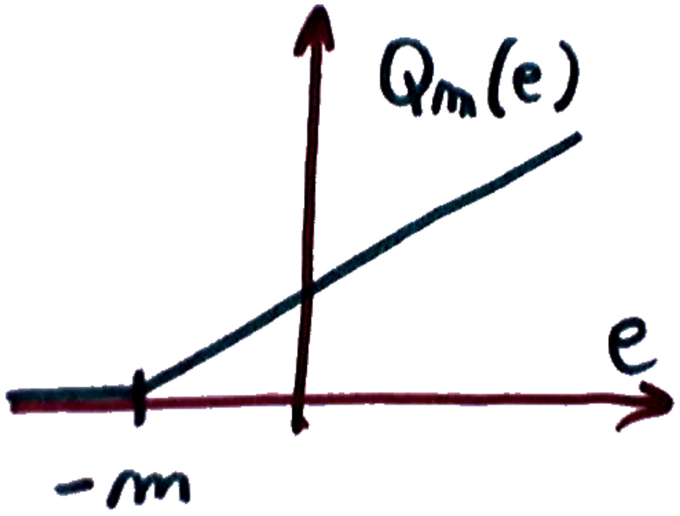
Adjust W so that $E(W, Y^i, X^i)$ gets smaller, while $\check{Y} = \min_{Y \in \{Y\}} E(W, Y, X^i)$ gets bigger (or more precisely, so that the difference decreases).
This algorithm makes no update whenever the energy of the desired Y is lower than all the others.

Examples of Loss: Margin Loss

Margin Loss: for discrete output set $\{Y\}$:

$$L_{\text{margin}}(W, Y^i, X^i) = Q_m\left(E(W, Y^i, X^i) - \min_{Y \in \{Y\}, Y \neq Y^i} E(W, Y, X^i)\right)$$

where $Q_m(e)$ is any function that is monotonically increasing for $e > -m$, where m is a constant called the **margin**.



Adjust W so that $E(W, Y^i, X^i)$ gets smaller, while all $E(W, Y, X^i)$ for which $E(W, Y, X^i) - E(W, Y^i, X^i) < m$ get bigger. This guarantees that the energy of the desired Y will be smaller than all other energies by at least m.

Examples of Loss: Log-Likelihood Loss

Log-Likelihood Loss:

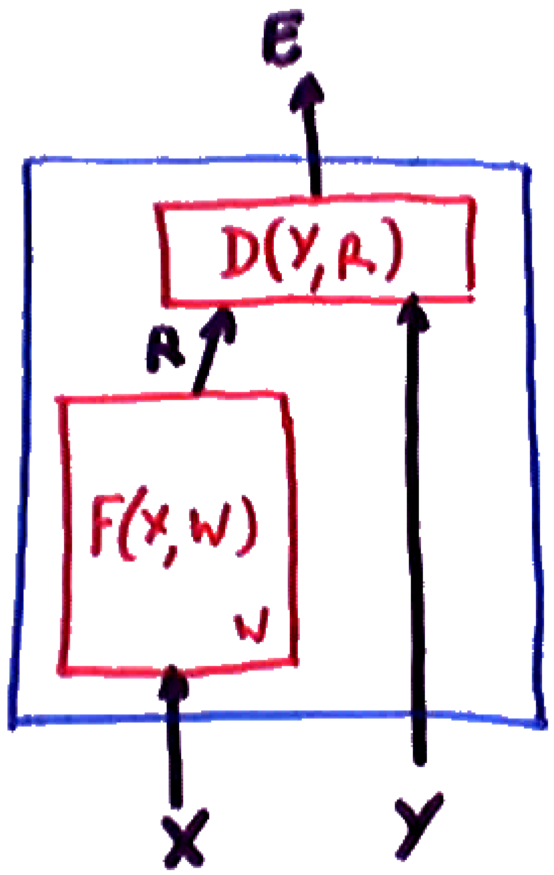
$$L_{\text{ll}}(W, Y^i, X^i) = E(W, Y^i, X^i) + \frac{1}{\beta} \log \left(\sum_{Y \in \{Y\}} \exp(-\beta E(W, Y, X^i)) \right)$$

where β is a positive constant.

- The function $\mathcal{F}_\beta(\{Y\}) = \frac{1}{\beta} \log \left(\sum_{Y \in \{Y\}} \exp(-\beta E(W, Y, X^i)) \right)$ is called the **free energy** of the ensemble $\{Y\}$ for temperature $1/\beta$.
- We define $\mathcal{Z}_\beta(\{Y\}) = \sum_{Y \in \{Y\}} \exp(-\beta E(W, Y, X^i))$ as the **partition function** of ensemble $\{Y\}$.
- Interesting property # 1: $\mathcal{F}_\beta(\{Y\}) = \frac{1}{\beta} \log \mathcal{Z}_\beta(\{Y\})$
- Interesting property # 2: $\lim_{\beta \to \infty} \mathcal{F}_\beta(\{Y\}) = \min_{Y \in \{Y\}} E(W, Y, X^i)$

For very large β, the log-likelihood loss reduces to the Perceptron loss.

Energy-Based Supervised Learning



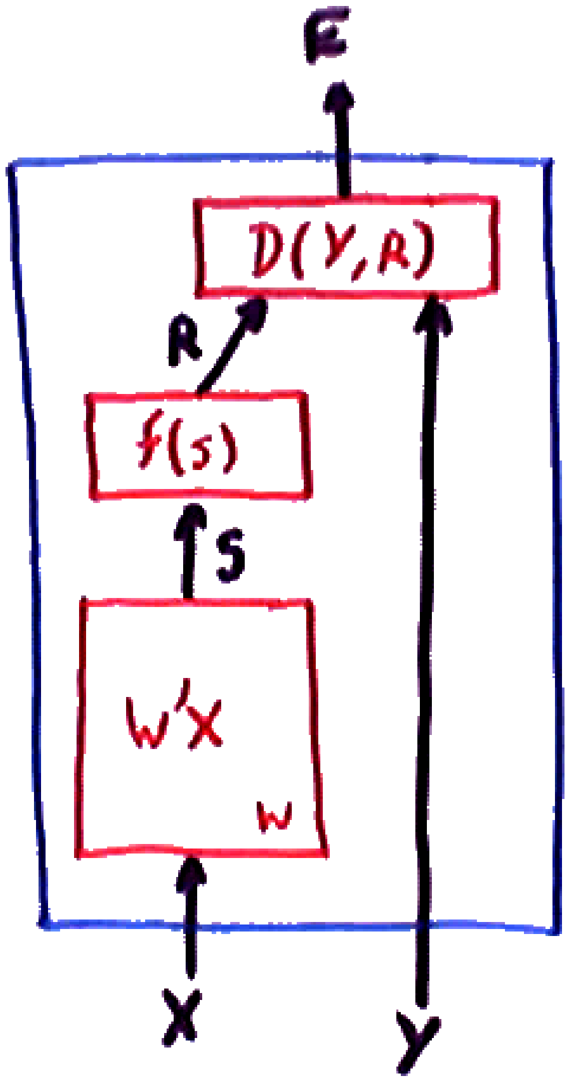
- A *supervised* system parameterizes $E(W, Y, X)$ as follows:

$$E(W, Y, X) = D(Y, F(W, X))$$

  where $F(W, X)$ is a suitably chosen *discriminant function* parameterized by W, and D is an appropriately chosen dissimilarity measure.
- A popular example would be

$$E(Y, X, W) = ||Y - F(X, W)||^2$$

Linear Machines



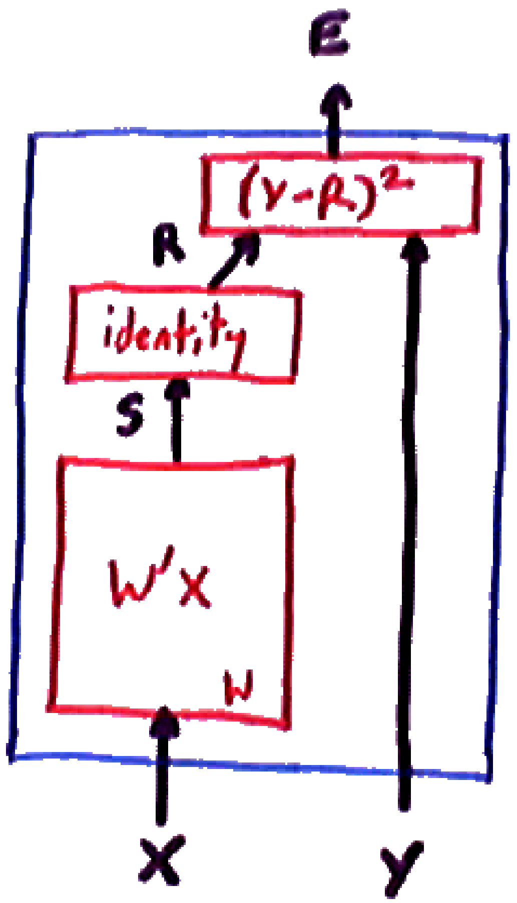
- The learning algorithms we have seen so far (perceptron, linear regression) are of that form, with the assumption that $G(W, X)$ only depends on the dot product of W and X.
- In other words, The E function of 2-class linear classifiers can be written as:

$$E(Y, X, W) = D(Y, f(W'X))$$

  where $W'X$ is the dot product of vectors W and X, and f is a monotonically increasing scalar function.
- in the following, we assume $Y = -1$ for class 1, and $Y = +1$ for class 2.

Linear Regression

Linear regression uses the Energy loss, or (equivalently) the Log-Likelihood loss.

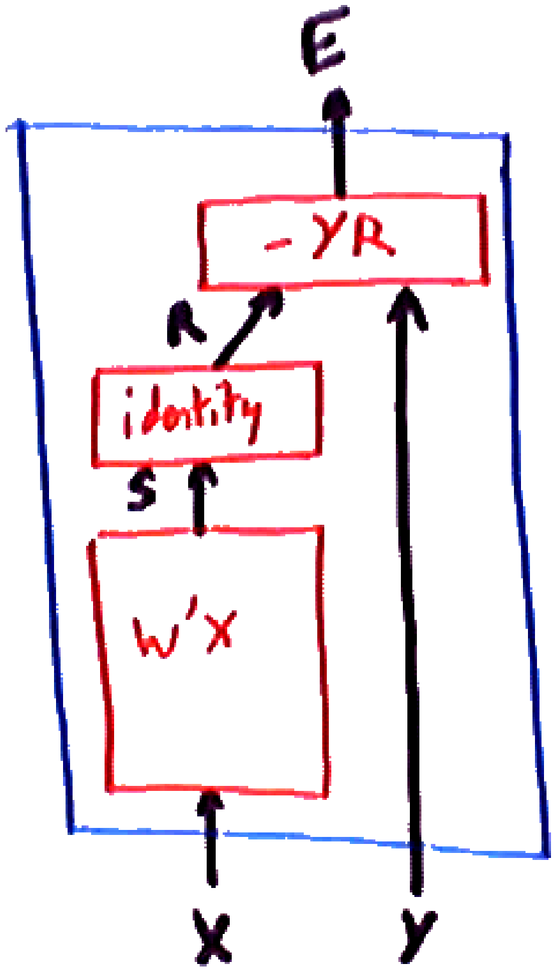


- $R = W'X$
- $E(W, Y, X) = D(Y, R) = \frac{1}{2}||Y - R||^2$
- $L(W, Y^i, X^i) = D(Y^i, W'X^i)$
- $\frac{\partial L}{\partial W} = \frac{\partial D(Y^i, R)}{\partial R} \frac{\partial R}{\partial W}$
- $\frac{\partial L}{\partial W} = \frac{\partial D(Y^i, R)}{\partial R} \frac{\partial (W'X^i)}{\partial W} = (R - Y^i)X^i$
- descent: $W \leftarrow W + \eta(Y^i - R)X^i$

Perceptron

$$L_{\text{perceptron}}(W, Y^i, X^i) = E(W, Y^i, X^i) - \min_{Y \in \{Y\}} E(W, Y, X^i)$$

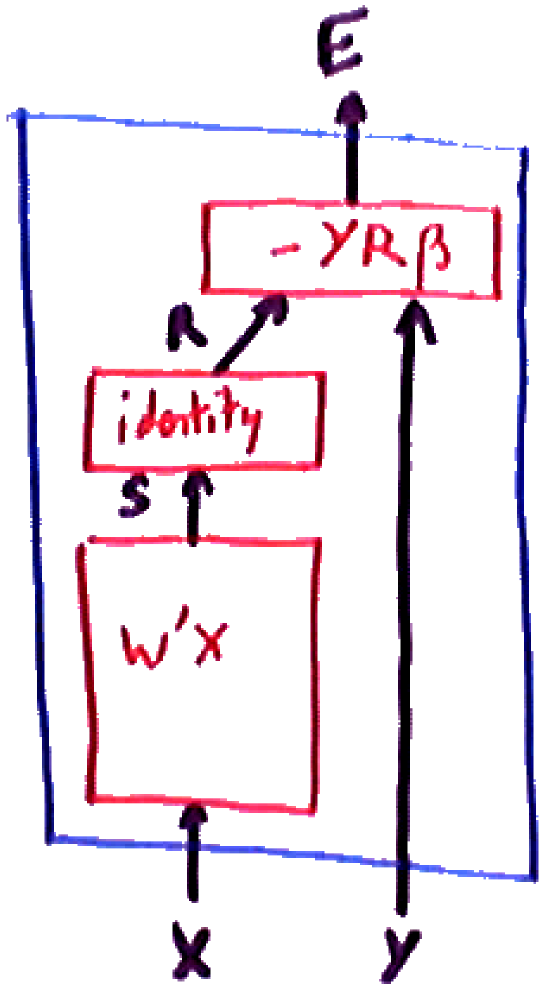
$\{Y\} = \{-1, +1\}$.



- $R = W'X$
- $E(Y, X, W) = D(Y, R) = -YR$
- $Y \in \{-1, +1\}$, hence $\min_Y -YR = -\text{sign}(R)R$ where $\text{sign}(R) = 1$ iff $R > 0$, and -1 otherwise.
- $L(W, Y^i, X^i) = -(Y^i - \text{sign}(R))R$
- $\frac{\partial L}{\partial W} = \frac{\partial -(Y^i - \text{sign}(R))R}{\partial R} \frac{\partial R}{\partial W}$
- $\frac{\partial L}{\partial W} = -(Y^i - \text{sign}(W'X^i))X^i$
- descent: $W \leftarrow W + \eta(Y^i - \text{sign}(W'X^i))X^i$

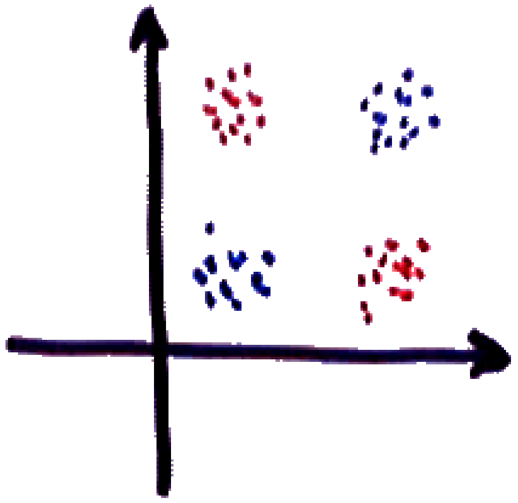
Logistic Regression

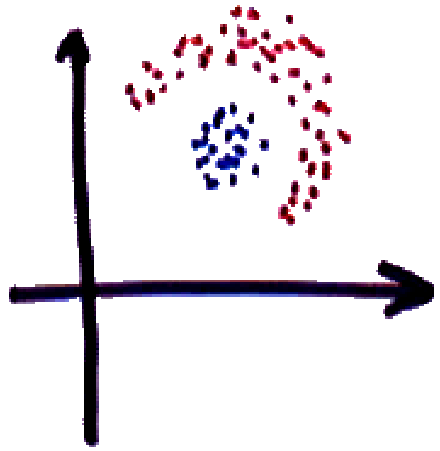
$$L_{\text{ll}}(W) = E(Y^i, X^i, W) + \log\left(\sum_{Y \in \{Y\}} \exp(-E(W, Y, X^i))\right)$$



- $R = \frac{1}{2} W'X$
- $E(Y, X, W) = D(Y, R) = -\frac{1}{2} Y R = -\frac{1}{2} Y W' X$
- $L(W) = \log(1 + \exp(-Y^i W' X^i))$
- $\frac{\partial L}{\partial W} = \frac{\partial D(Y^i, R)}{\partial R} \frac{\partial S}{\partial W}$
- $\frac{\partial L}{\partial W} = -\left(\frac{Y^i+1}{2} - \frac{1}{1+\exp(-W'X^i)}\right) X^i$
- descent: $W \leftarrow W + \eta \left(\frac{Y^i+1}{2} - \frac{1}{1+\exp(-W'X^i)}\right) X^i$

Limitations of Linear Machines

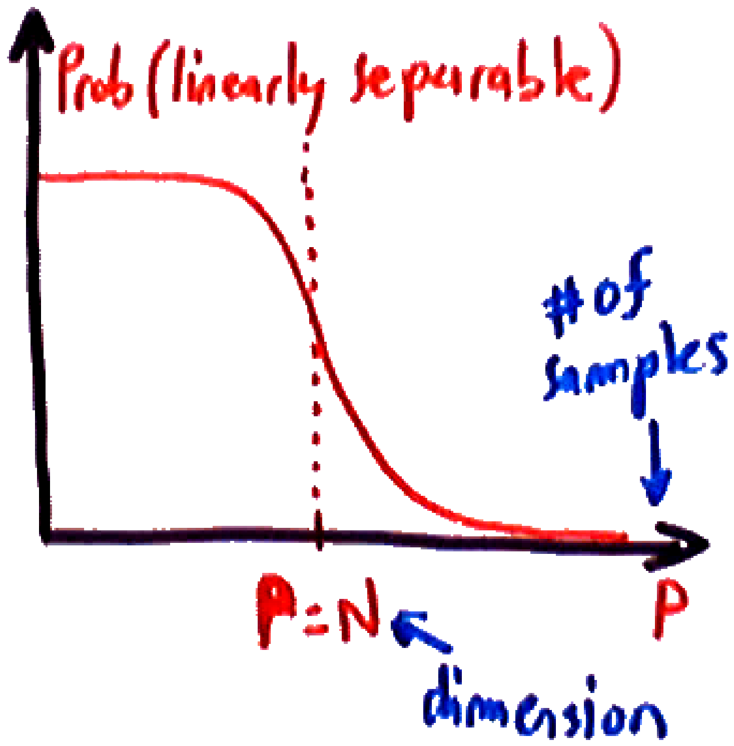




The *Linearly separable* dichotomies are the partitions that are realizable by a linear classifier (the boundary between the classes is a hyperplane).

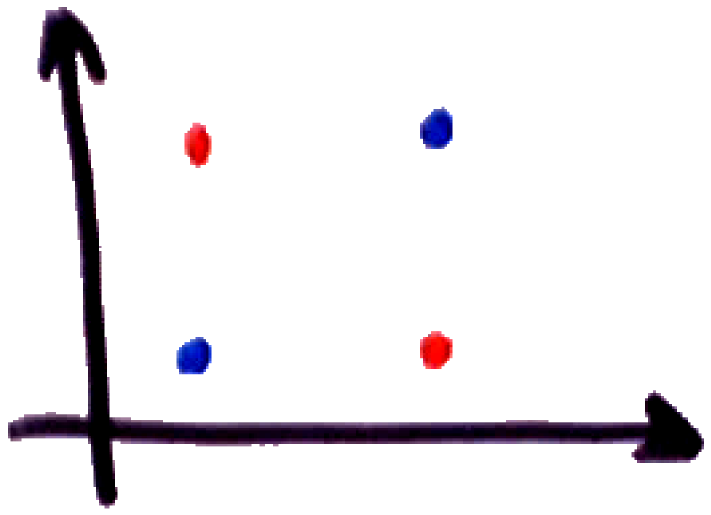
Number of Linearly Separable Dichotomies

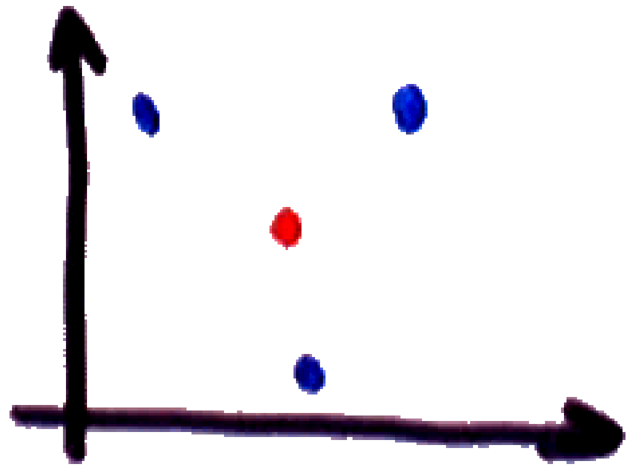
The probability that P samples of dimension N are linearly separable goes to zero very quickly as P grows larger than N (Cover's theorem, 1966).



- Problem: there are 2^P possible dichotomies of P points.
- Only about N are linearly separable.
- If P is larger than N, the probability that a random dichotomy is linearly separable is very, very small.

Example of Non-Linearly Separable Dichotomies





- Some seemingly simple dichotomies are not linearly separable
- Question: How do we make a given problem linearly separable?