Energy-Based Learning

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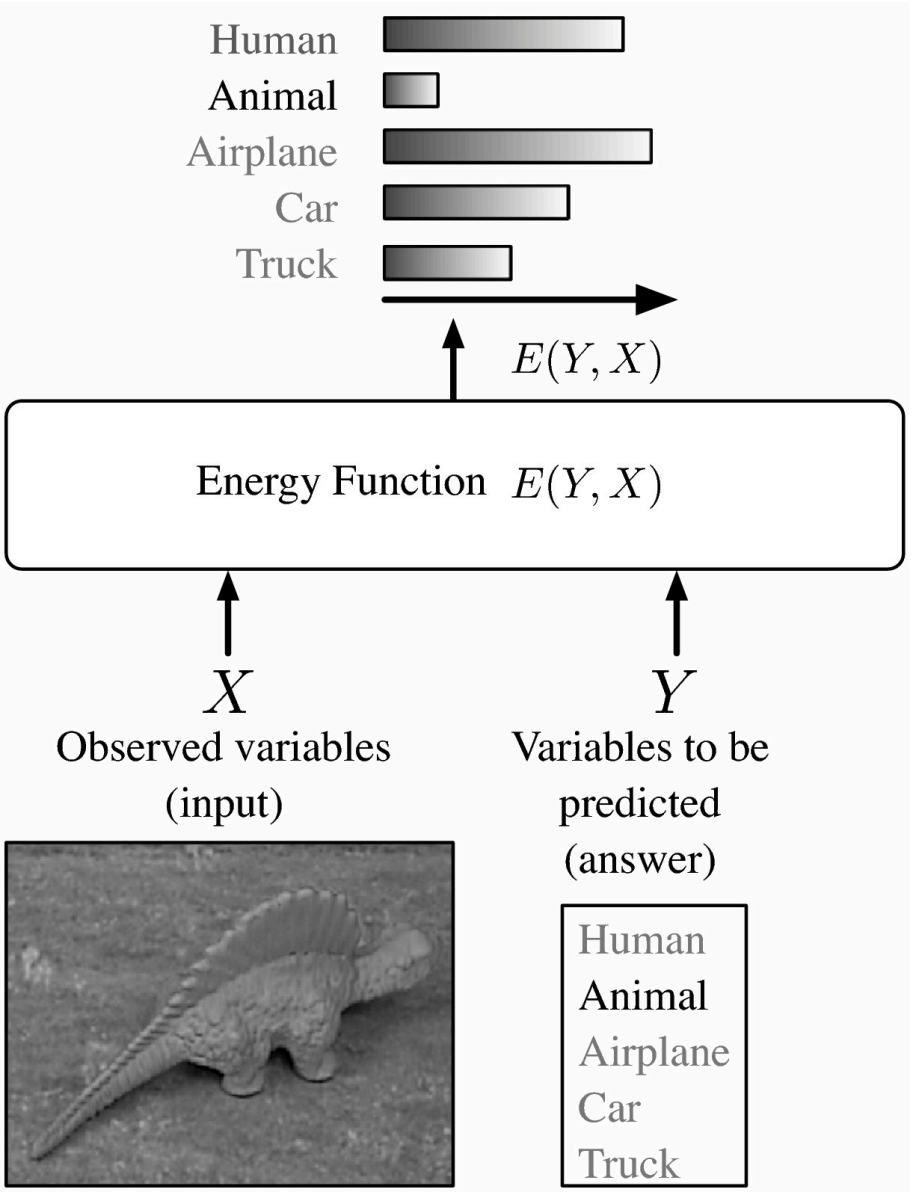
Energy-Based Model for Decision-Making



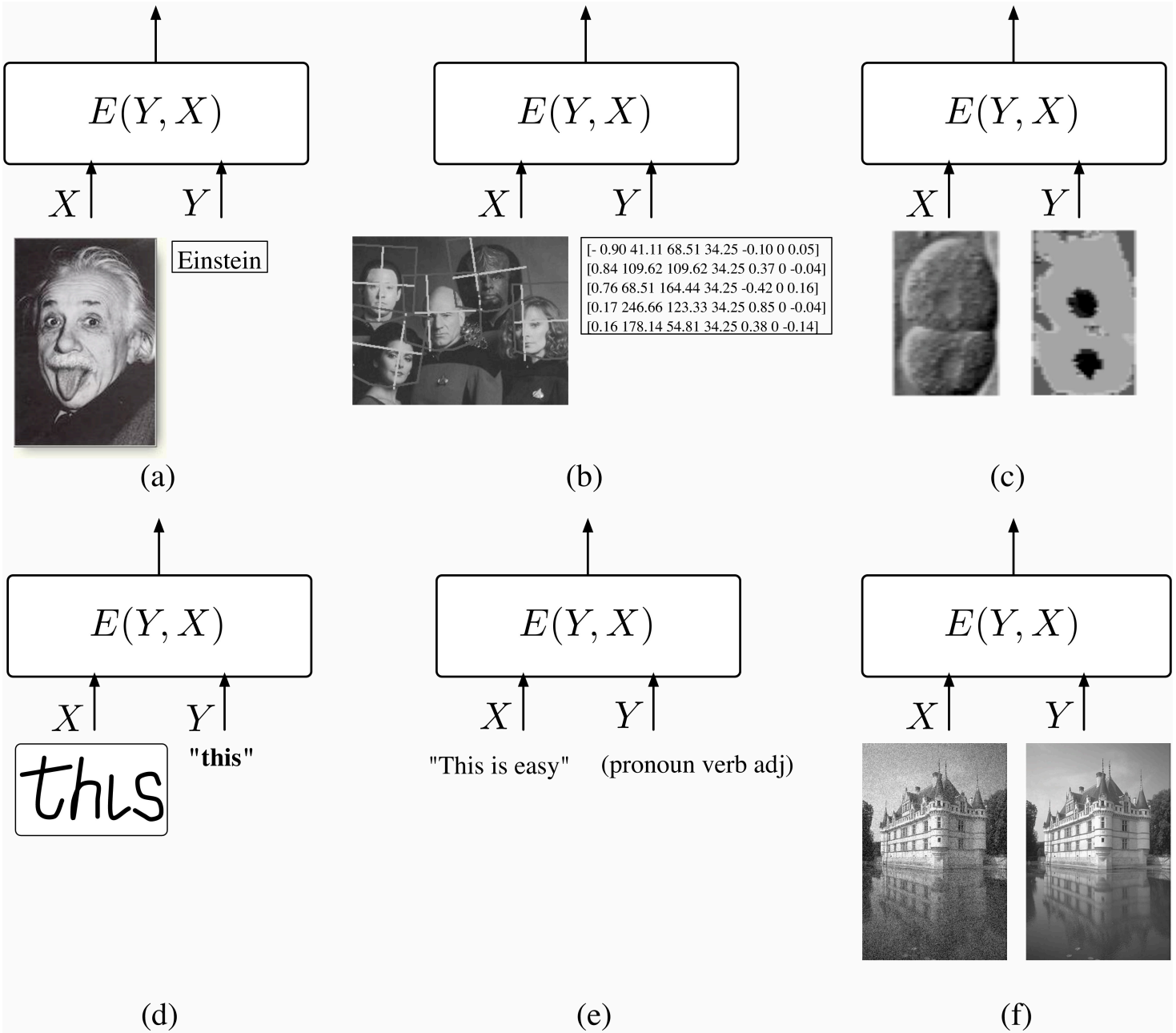
Model: **Measures the compatibility between an observed variable X and a variable to be predicted Y through an energy function E(Y,X).**

$$Y^* = \text{argmin}_{Y \in \mathcal{Y}} E(Y, X).$$

Inference: **Search for the Y that minimizes the energy within a set $\mathcal{Y}$**

If the set has low cardinality, we can use exhaustive search.

Complex Tasks: Inference is non-trivial



When the cardinality or dimension of Y is large, exhaustive search is impractical.

We need to use a "smart" inference procedure: min-sum, Viterbi, ...

What Questions Can a Model Answer?

1. Classification & Decision Making:

"which value of Y is most compatible with X?"

Applications: Robot navigation,.....

Training: give the lowest energy to the correct answer

2. Ranking:

"Is Y1 or Y2 more compatible with X?"

Applications: Data-mining....

Training: produce energies that rank the answers correctly

3. Detection:

"Is this value of Y compatible with X"?

Application: face detection....

Training: energies that increase as the image looks less like a face.

4. Conditional Density Estimation:

"What is the conditional distribution P(Y|X)?"

Application: feeding a decision-making system

Training: differences of energies must be just so.

Decision-Making versus Probabilistic Modeling

Energies are uncalibrated

The energies of two separately-trained systems cannot be combined

The energies are uncalibrated (measured in arbitrary untis)

How do we calibrate energies?

We turn them into probabilities (positive numbers that sum to 1).

Simplest way: Gibbs distribution

Other ways can be reduced to Gibbs by a suitable redefinition of the energy.

$$P(Y|X) = \frac{e^{-\beta E(Y,X)}}{\int_{y \in \mathcal{Y}} e^{-\beta E(y,X)}},$$

Partition function

Inverse temperature

Architecture and Loss Function

Family of energy functions $\mathcal{E} = \{E(W, Y, X) : \quad W \in \mathcal{W}\}.$

Training set $\mathcal{S} = \{(X^i, Y^i) : i = 1 \ldots P\}$

Loss functional / Loss function $\mathcal{L}(E, \mathcal{S}) \qquad \mathcal{L}(W, \mathcal{S})$

Measures the quality of an energy function

Training $W^* = \min_{W \in \mathcal{W}} \mathcal{L}(W, \mathcal{S}).$

Form of the loss functional

invariant under permutations and repetitions of the samples

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

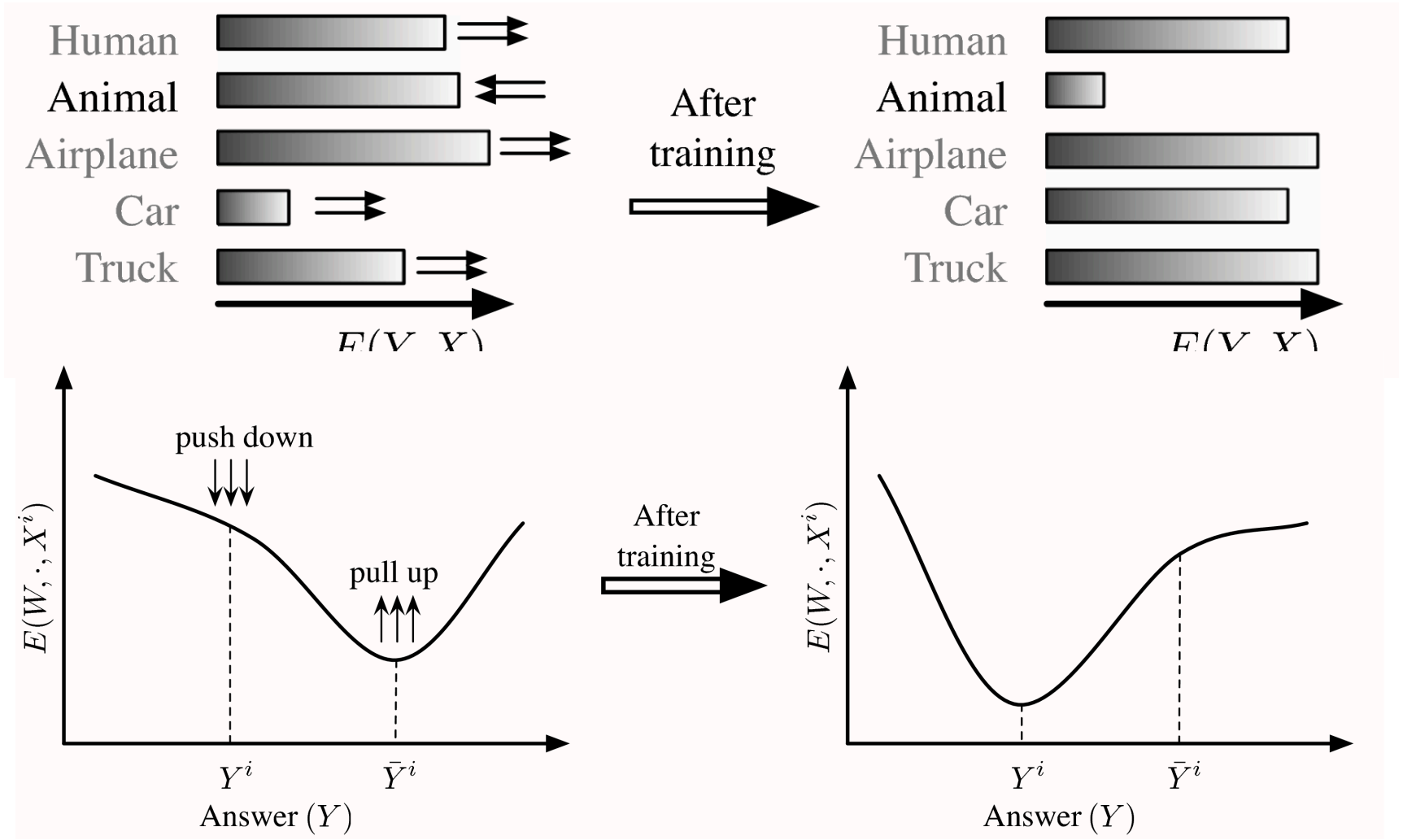
Per-sample loss

Desired answer

Energy surface for a given Xi as Y varies

Regularizer

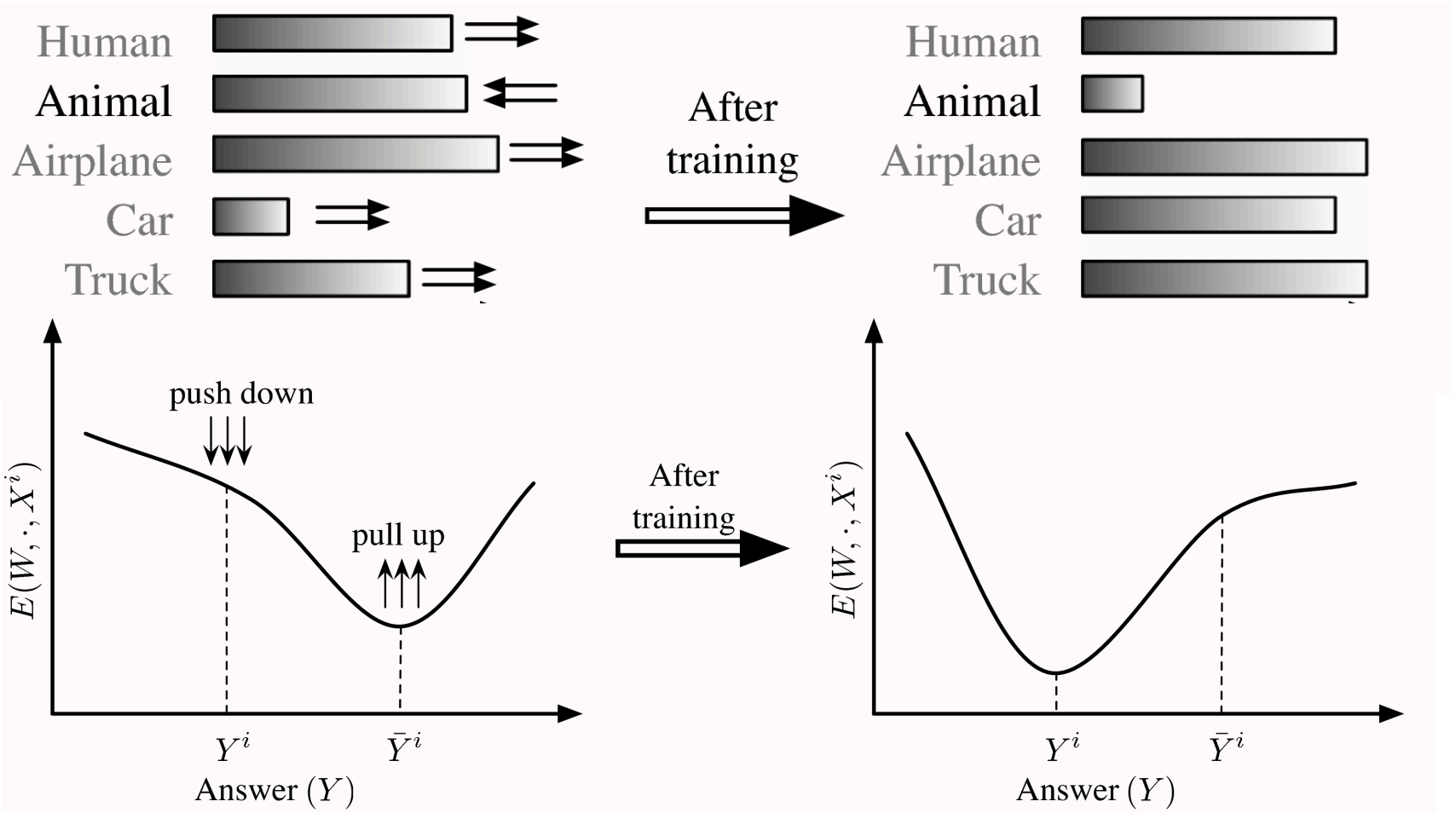
Designing a Loss Functional



Correct answer has the lowest energy -> LOW LOSS

Lowest energy is not for the correct answer -> HIGH LOSS

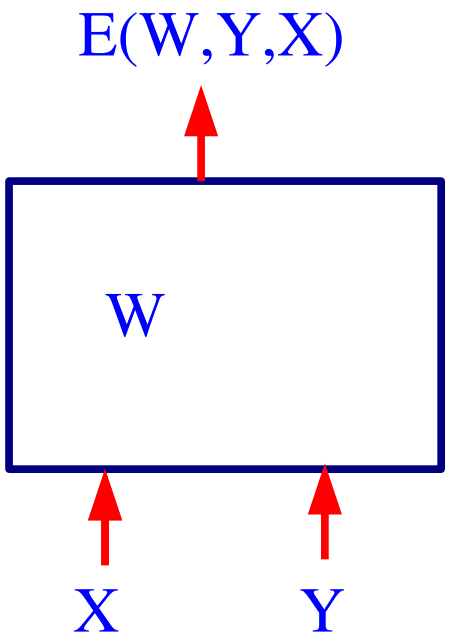
Designing a Loss Functional



Push down on the energy of the correct answer

Pull up on the energies of the incorrect answers, particularly if they are smaller than the correct one

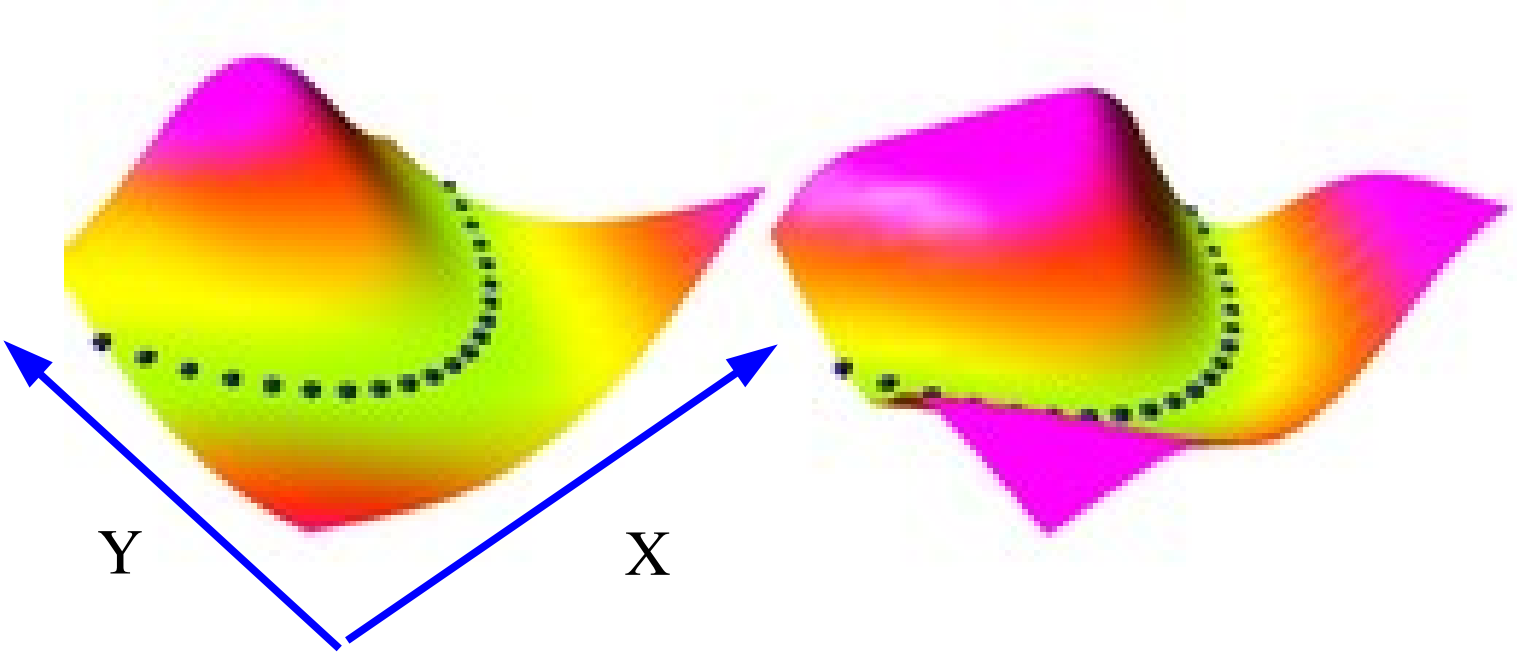
Architecture + Inference Algo + Loss Function = Model



1. **Design an architecture:** a particular form for E(W,Y,X).
2. **Pick an inference algorithm for Y:** MAP or conditional distribution, belief prop, min cut, variational methods, gradient descent, MCMC, HMC.....
3. **Pick a loss function:** in such a way that minimizing it with respect to W over a training set will make the inference algorithm find the correct Y for a given X.
4. **Pick an optimization method.**

PROBLEM: What loss functions will make the machine approach the desired behavior?

Several Energy Surfaces can give the same answers

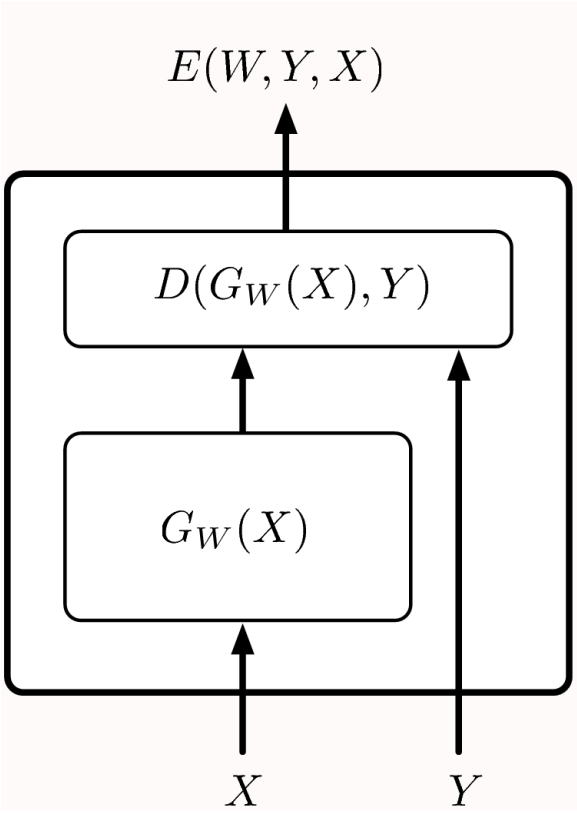


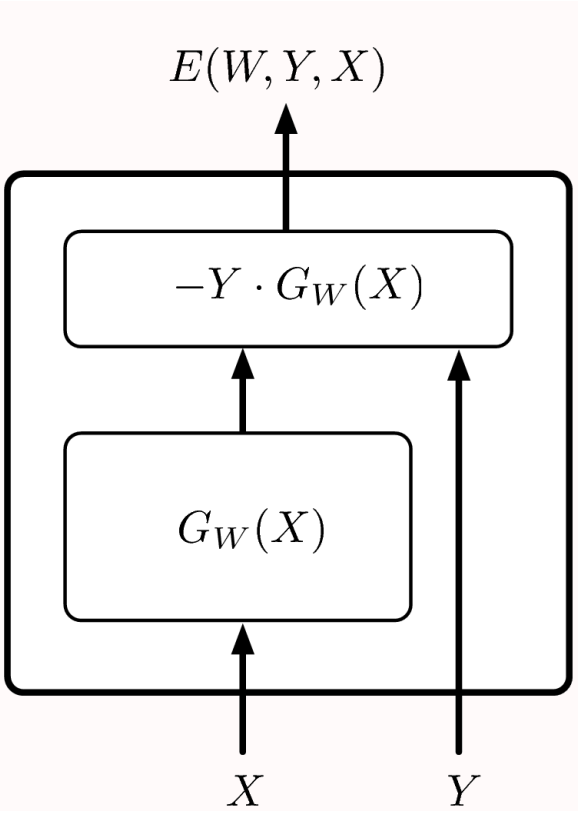
Both surfaces compute Y=X^2

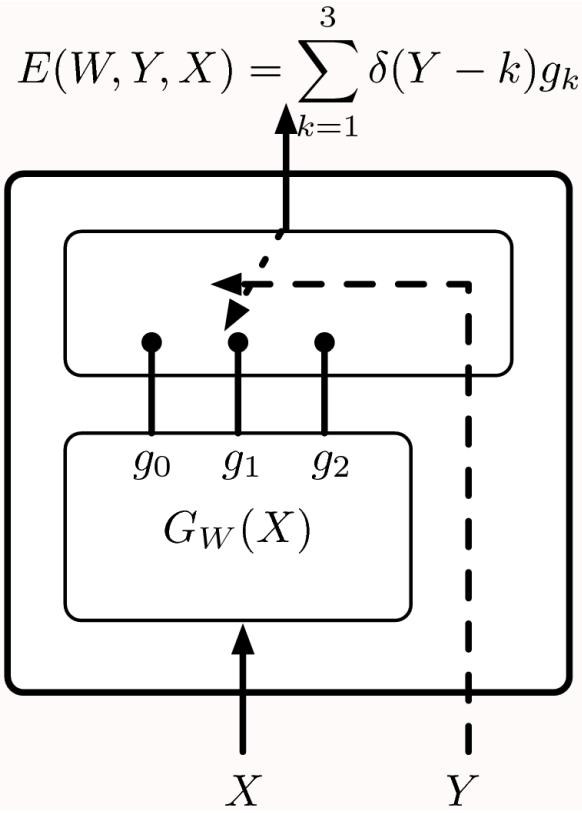
MINy E(Y,X) = X^2

Minimum-energy inference gives us the same answer

Simple Architectures







Regression

$$E(W,Y,X) = \frac{1}{2}||G_W(X) - Y||^2.$$

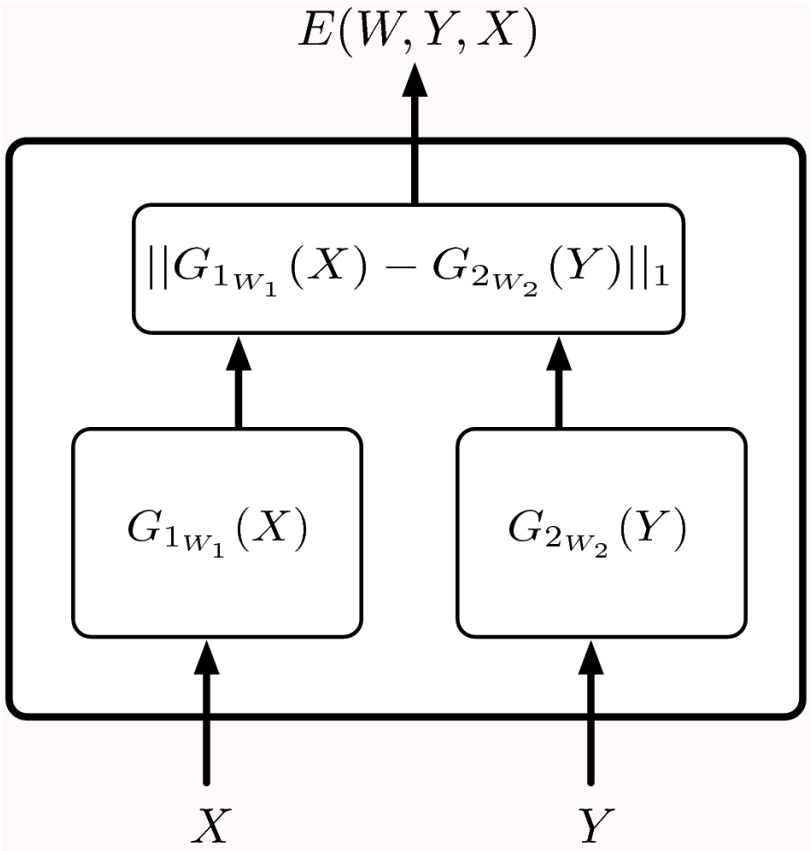
Binary Classification

$$E(W,Y,X) = -Y G_W(X),$$

Multi-class Classification

Simple Architecture: Implicit Regression

$$E(W, X, Y) = ||G_{1_{W_1}}(X) - G_{2_{W_2}}(Y)||_1,$$



The Implicit Regression architecture

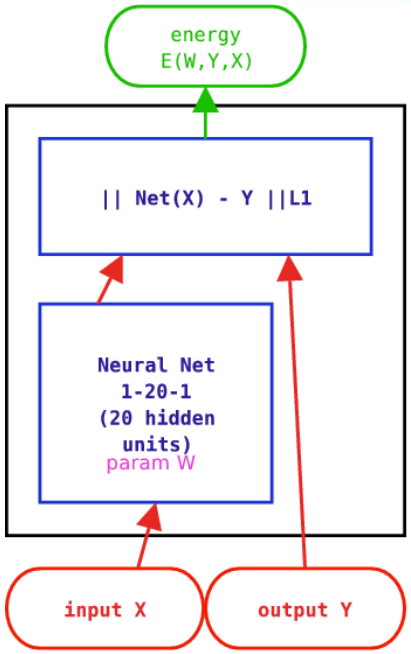
- allows multiple answers to have low energy.
- Encodes a constraint between X and Y rather than an explicit functional relationship
- This is useful for many applications
- Example: sentence completion: "The cat ate the {mouse,bird,homework,...}"
- [Bengio et al. 2003]
- But, inference may be difficult.

Examples of Loss Functions: Energy Loss

Energy Loss $$L_{energy}(Y^i, E(W, \mathcal{Y}, X^i)) = E(W, Y^i, X^i).$$

Simply pushes down on the energy of the correct answer

WORKS!!!



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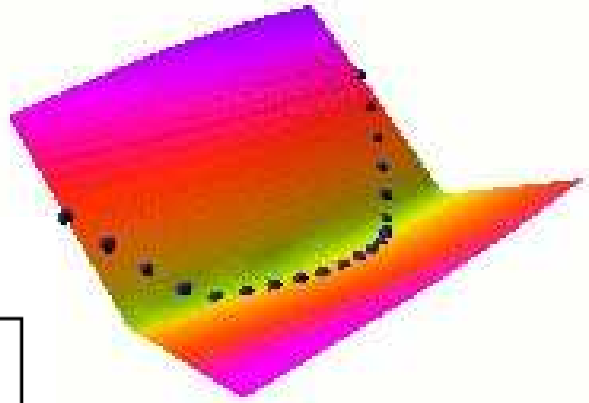
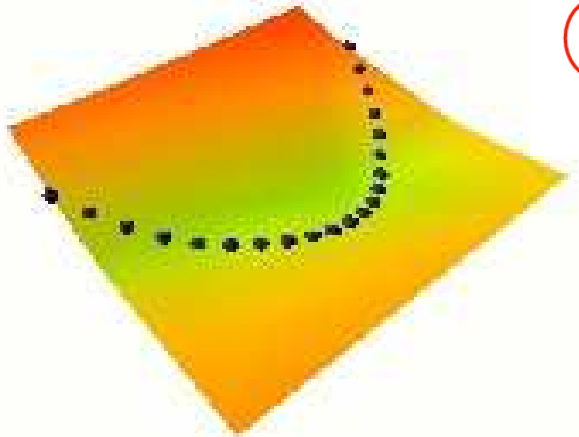
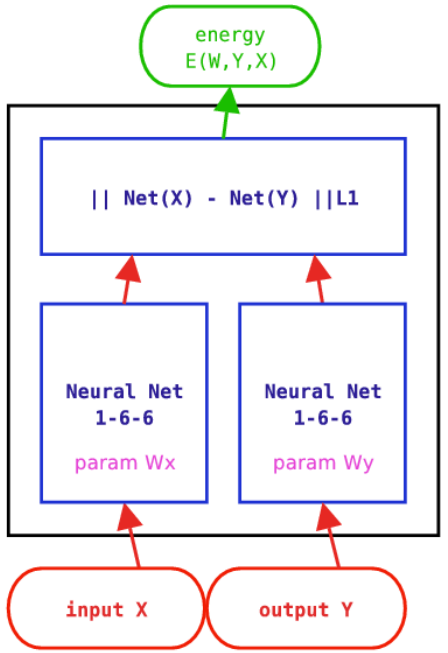






(b)

COLLAPSES!!!

Examples of Loss Functions:Perceptron Loss

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

Perceptron Loss

- Pushes down on the energy of the correct answer
- Pulls up on the energy of the machine's answer
- Always positive. Zero when answer is correct
- No "margin": technically does not prevent the energy surface from being almost flat.
- Works pretty well in practice, particularly if the energy parameterization does not allow flat surfaces.

Perceptron Loss for Binary Classification

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

Energy: $$E(W, Y, X) = -Y G_W(X),$$

Inference: $$Y^* = \text{argmin}_{Y \in \{-1,1\}} - Y G_W(X) = \text{sign}(G_W(X)).$$

Loss: $$\mathcal{L}_{\text{perceptron}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \left(\text{sign}(G_W(X^i)) - Y^i\right) G_W(X^i).$$

Learning Rule: $$W \leftarrow W + \eta \left(Y^i - \text{sign}(G_W(X^i))\right) \frac{\partial G_W(X^i)}{\partial W},$$

If Gw(X) is linear in W: $$E(W, Y, X) = -Y W^T \Phi(X)$$

$$W \leftarrow W + \eta \left(Y^i - \text{sign}(W^T \Phi(X^i))\right) \Phi(X^i)$$

Examples of Loss Functions: Generalized Margin Losses

First, we need to define the Most Offending Incorrect Answer

Most Offending Incorrect Answer: discrete case

Definition 1 *Let Y be a discrete variable. Then for a training sample (X^i, Y^i), the* ***most offending incorrect answer*** $\bar{Y}^i$ *is the answer that has the lowest energy among all answers that are incorrect:*

$$\bar{Y}^i = \text{argmin}_{Y \in \mathcal{Y} and Y \neq Y^i} E(W, Y, X^i). \quad (8)$$

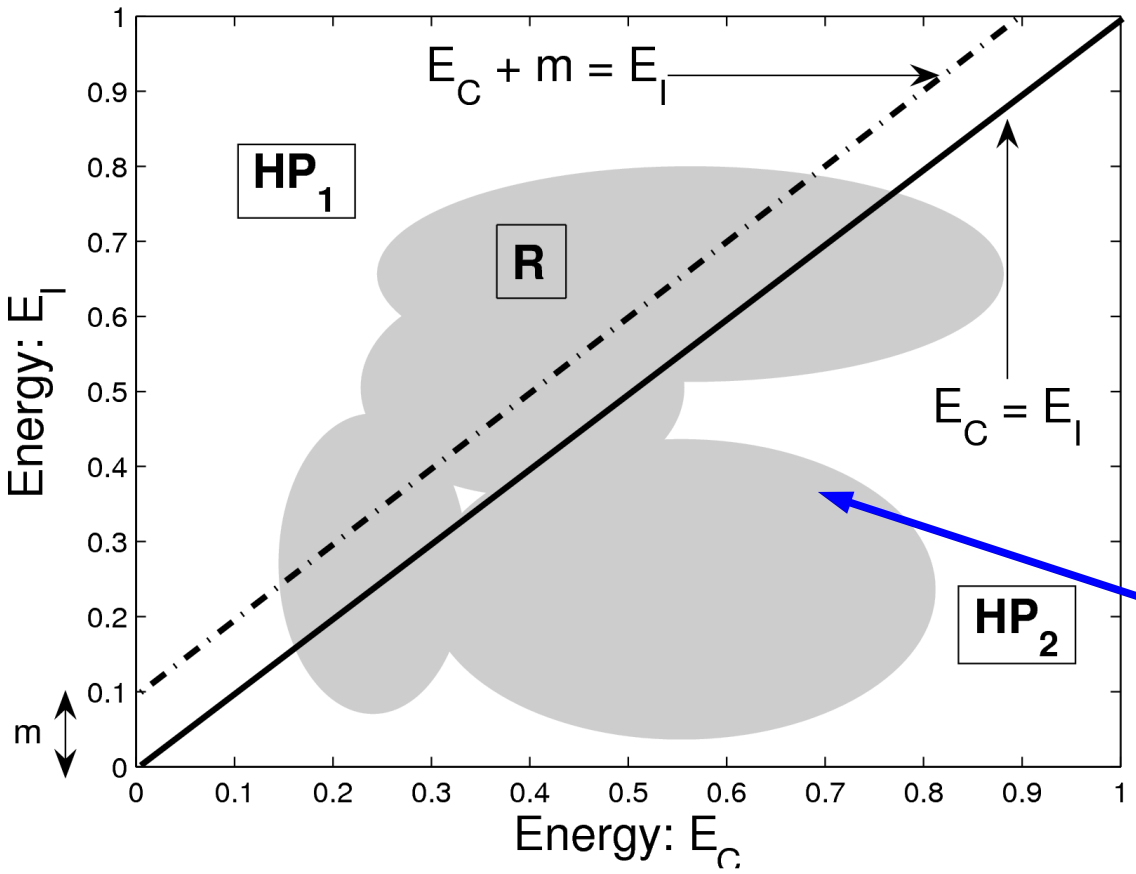
Most Offending Incorrect Answer: continuous case

Definition 2 *Let Y be a continuous variable. Then for a training sample (X^i, Y^i), the* ***most offending incorrect answer*** $\bar{Y}^i$ *is the answer that has the lowest energy among all answers that are at least ϵ away from the correct answer:*

$$\bar{Y}^i = \text{argmin}_{Y \in \mathcal{Y}, \|Y - Y^i\| > \epsilon} E(W, Y, X^i). \quad (9)$$

Examples of Loss Functions: Generalized Margin Losses

$$L_{\text{margin}}(W, Y^i, X^i) = Q_m\left(E(W, Y^i, X^i), E(W, \bar{Y}^i, X^i)\right).$$



Generalized Margin Loss

Qm increases with the energy of the correct answer

Qm decreases with the energy of the most offending incorrect answer

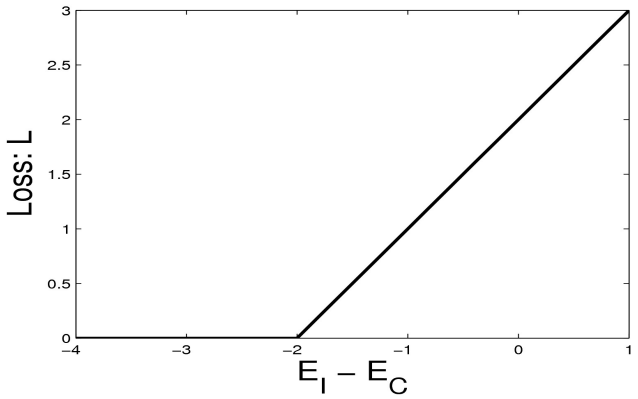
whenever it is less than the energy of the correct answer plus a margin m.

Examples of Generalized Margin Losses

$$L_{\text{hinge}}(W, Y^i, X^i) = \max\left(0, m + E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right),$$

Hinge Loss

With the linearly-parameterized binary classifier architecture, we get linear SV

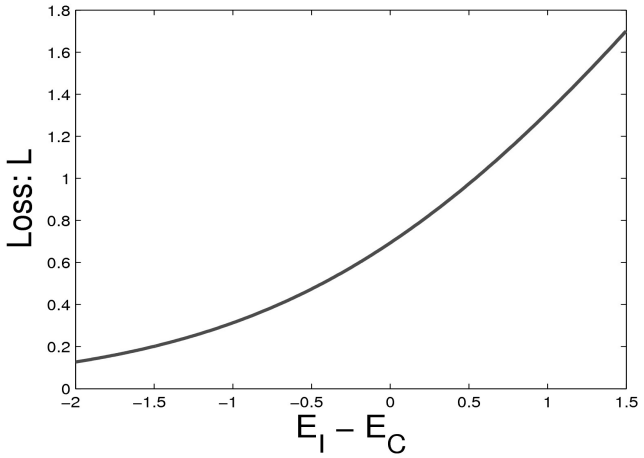


$$L_{\text{log}}(W, Y^i, X^i) = \log\left(1 + e^{E(W,Y^i,X^i) - E(W,\bar{Y}^i,X^i)}\right).$$

Log Loss

"soft hinge" loss

With the linearly-parameterized binary classifier architecture, we get linear Logistic Regression



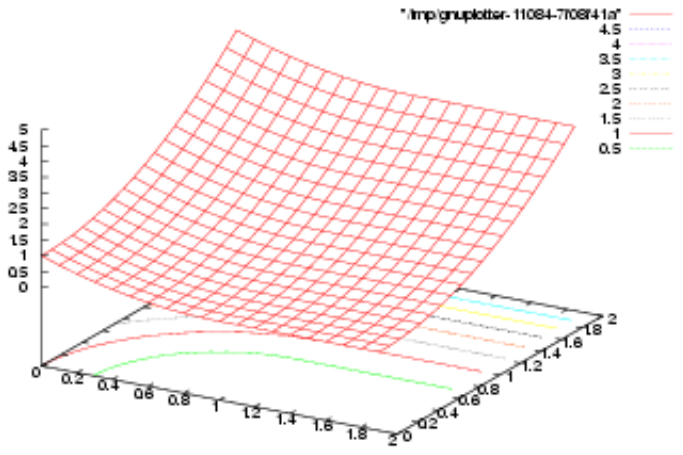
Examples of Margin Losses: Square-Square Loss

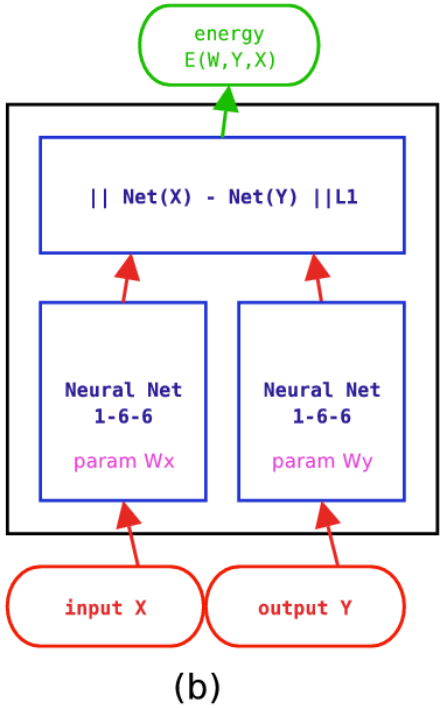
$$L_{\text{sq-sq}}(W, Y^i, X^i) = E(W, Y^i, X^i)^2 + \left(\max(0, m - E(W, \bar{Y}^i, X^i))\right)^2 .$$

Square-Square Loss

[LeCun-Huang 2005]

Appropriate for positive energy functions





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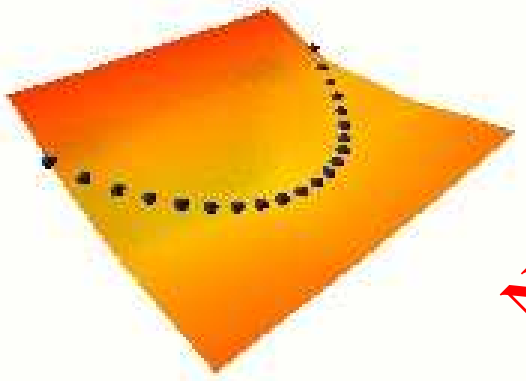
Learning Y = X^2



NO COLLAPSE!!!

Other Margin-Like Losses

LVQ2 Loss [Kohonen, Oja], Driancourt-Bottou 1991]

$$L_{\text{lvq2}}(W, Y^i, X^i) = \min\left(1, \max\left(0, \frac{E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)}{\delta E(W, \bar{Y}^i, X^i)}\right)\right),$$

Minimum Classification Error Loss [Juang, Chou, Lee 1997]

$$L_{\text{mce}}(W, Y^i, X^i) = \sigma\left(E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right),$$

$$\sigma(x) = (1 + e^{-x})^{-1}$$

Square-Exponential Loss [Osadchy, Miller, LeCun 2004]

$$L_{\text{sq-exp}}(W, Y^i, X^i) = E(W, Y^i, X^i)^2 + \gamma e^{-E(W, \bar{Y}^i, X^i)},$$

Negative Log-Likelihood Loss

Conditional probability of the samples (assuming independence)

$$P(Y^1, \ldots, Y^P | X^1, \ldots, X^P, W) = \prod_{i=1}^{P} P(Y^i | X^i, W).$$

$$-\log \prod_{i=1}^{P} P(Y^i | X^i, W) = \sum_{i=1}^{P} -\log P(Y^i | X^i, W).$$

Gibbs distribution: $$P(Y | X^i, W) = \frac{e^{-\beta E(W, Y, X^i)}}{\int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^i)}}.$$

$$-\log \prod_{i=1}^{P} P(Y^i | X^i, W) = \sum_{i=1}^{P} \beta E(W, Y^i, X^i) + \log \int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^i)}.$$

We get the NLL loss by dividing by P and Beta:

$$\mathcal{L}_{\text{nll}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \left(E(W, Y^i, X^i) + \frac{1}{\beta} \log \int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^i)} \right).$$

Reduces to the perceptron loss when Beta->infinity

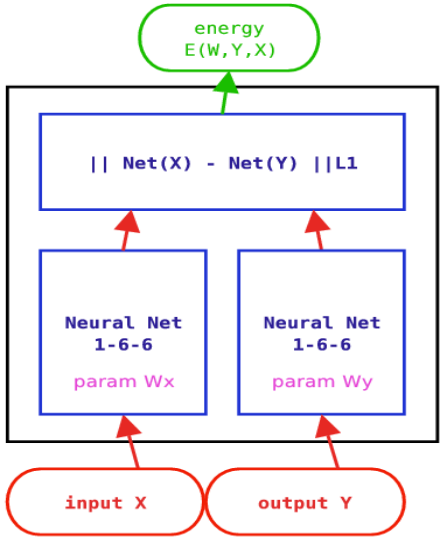
Negative Log-Likelihood Loss

Pushes down on the energy of the correct answer

Pulls up on the energies of all answers in proportion to their probability

$$\mathcal{L}_{\text{nll}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \left(E(W, Y^i, X^i) + \frac{1}{\beta} \log \int_{y \in \mathcal{Y}} e^{-\beta E(W, y, X^i)} \right).$$

$$\frac{\partial L_{\text{nll}}(W, Y^i, X^i)}{\partial W} = \frac{\partial E(W, Y^i, X^i)}{\partial W} - \int_{Y \in \mathcal{Y}} \frac{\partial E(W, Y, X^i)}{\partial W} P(Y | X^i, W),$$



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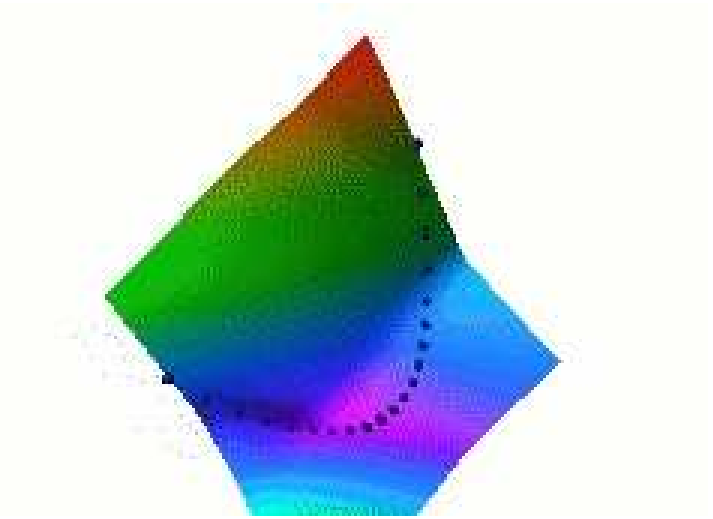


Negative Log-Likelihood Loss: Binary Classification

Binary Classifier Architecture:

$$\mathcal{L}_{\text{nll}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \left[-Y^i G_W(X^i) + \log \left(e^{Y^i G_W(X^i)} + e^{-Y^i G_W(X^i)} \right) \right].$$

$$\mathcal{L}_{\text{nll}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \log \left(1 + e^{-2Y^i G_W(X^i)} \right),$$

Linear Binary Classifier Architecture:

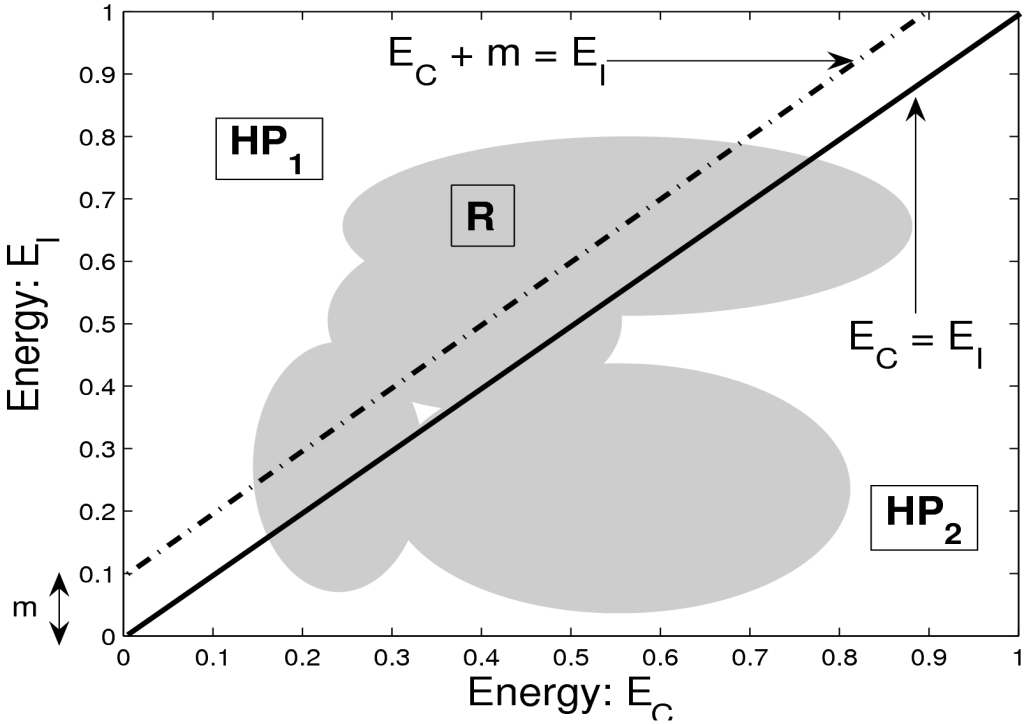
$$\mathcal{L}_{\text{nll}}(W, \mathcal{S}) = \frac{1}{P} \sum_{i=1}^{P} \log \left(1 + e^{-2Y^i W^T \Phi(X^i)} \right).$$

Learning Rule: logistic regression

What Makes a "Good" Loss Function

Good loss functions make the machine produce the correct answer

Avoid collapses and flat energy surfaces



Sufficient Condition on the Loss

Let (X^i, Y^i) be the i^{th} training example and m be a positive margin. Minimizing the loss function L will cause the machine to satisfy $E(W, Y^i, X^i) < E(W, Y, X^i) - m$ for all $Y \neq Y^i$, if there exists at least one point (e_1, e_2) with $e_1 + m < e_2$ such that for all points (e'_1, e'_2) with $e'_1 + m \geq e'_2$, we have

$$Q_{[E_y]}(e_1, e_2) < Q_{[E_y]}(e'_1, e'_2),$$

where $Q_{[E_y]}$ is given by

$$L(W, Y^i, X^i) = Q_{[E_y]}(E(W, Y^i, X^i), E(W, \bar{Y}^i, X^i)).$$

What Make a "Good" Loss Function

Good and bad loss functions

Loss (equation #)	Formula	Margin
energy loss	$E(W, Y^i, X^i)$	none
perceptron	$E(W, Y^i, X^i) - \min_{Y \in \mathcal{Y}} E(W, Y, X^i)$	0
hinge	$\max\left(0, m + E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right)$	m
log	$\log\left(1 + e^{E(W,Y^i,X^i) - E(W,\bar{Y}^i,X^i)}\right)$	> 0
LVQ2	$\min\left(M, \max(0, E(W, Y^i, X^i) - E(W, \bar{Y}^i, X^i)\right)$	0
MCE	$\left(1 + e^{-\left(E(W,Y^i,X^i) - E(W,\bar{Y}^i,X^i)\right)}\right)^{-1}$	> 0
square-square	$E(W, Y^i, X^i)^2 - \left(\max(0, m - E(W, \bar{Y}^i, X^i))\right)^2$	m
square-exp	$E(W, Y^i, X^i)^2 + \beta e^{-E(W,\bar{Y}^i,X^i)}$	> 0
NLL/MMI	$E(W, Y^i, X^i) + \frac{1}{\beta} \log \int_{y \in \mathcal{Y}} e^{-\beta E(W,y,X^i)}$	> 0
MEE	$1 - e^{-\beta E(W,Y^i,X^i)} / \int_{y \in \mathcal{Y}} e^{-\beta E(W,y,X^i)}$	> 0

Advantages/Disadvantages of various losses

Loss functions differ in how they pick the point(s) whose energy is pulled up, and how much they pull them up

Losses with a log partition function in the contrastive term pull up all the bad answers simultaneously.

This may be good if the gradient of the contrastive term can be computed efficiently

This may be bad if it cannot, in which case we might as well use a loss with a single point in the contrastive term

Variational methods pull up many points, but not as many as with the full log partition function.

Efficiency of a loss/architecture: how many energies are pulled up for a given amount of computation?

The theory for this is to be developed