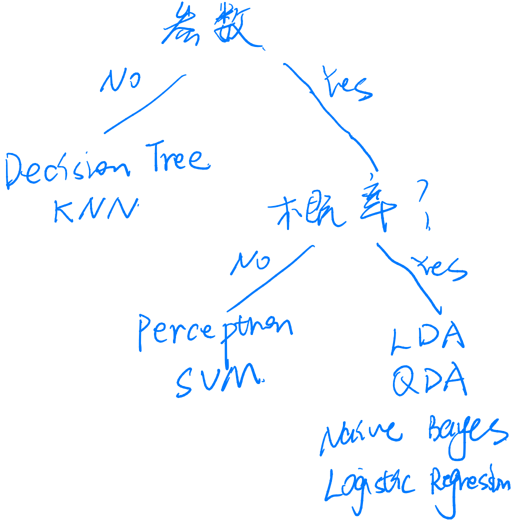
Linear Models for Classification

Table of contents



Section 1

Introduction

Classification: Definition

- Given a collection of records (training set)
  - Each record $(\mathbf{x}, y)$ contains a set of attributes/features/feature variables denoted as $\mathbf{x} \in \mathbb{R}^d$, and one target variable called class $y \in \{0, 1, \ldots, K-1\}$.
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- Goal: previously unseen records should be assigned a class as accurately as possible.
  - A test set is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with training set used to build the model and test set used to validate it.

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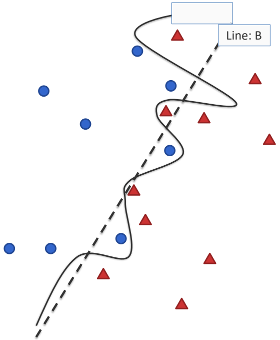
      Example: Representing $p(y = k|\mathbf{x})$ as parametric models and then optimizing the parameters using a training set
    - Generative method
      Model the class-conditional densities $p(\mathbf{x}|y = k)$ and prior probabilities $p(y = k)$, and compute $p(y = k|\mathbf{x})$ using Bayes theorem

$$p(y = k|\mathbf{x}) = \frac{p(\mathbf{x}|y = k)p(y = k)}{p(\mathbf{x})}$$

Decision Boundary

In the most common scenario, the classes are taken to be disjoint, so that each input $(\mathbf{x})$ is assigned to **one and only one class** (y).

- The input space is thereby divided into *decision regions* whose boundaries are called **decision boundaries** or **decision surfaces**.



- **Curve: A** and **Line: B** are decision boundaries for two different classifiers.
- The decision boundary **Line : B** is linear.

In the next few lectures, we consider classification models with linear decision boundaries.

Section 2

Perceptron

Case Study: Credit Approval

age	32 years
gender	male
salary	$40,000$
debt	$26,000$
years in job	1 year
years at home	3 years
...	...

Approve for credit?

- Using salary, debt, years in residence, etc. approve for credit or not
- Banks have lots of data
  - customer information: salary, debt, etc.
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- For convenience, instead of $y \in \{0, 1\}$, sometimes, we use $y \in \{-1, +1\}$ to denote the two classes.

A Simple Model: Linear Threshold Units

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- How to choose the importance weights w_i?
  - x_i is important $\Rightarrow$ large weight
  - x_i is beneficial for credit $\Rightarrow$ positive weight
  - x_i is detrimental for credit $\Rightarrow$ negative weight

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$$y(\mathbf{x}) = \mathrm{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) + w_0\right)$$

where w_0 is the "bias weight". The "bias weight" w_0 correspond to the threshold.

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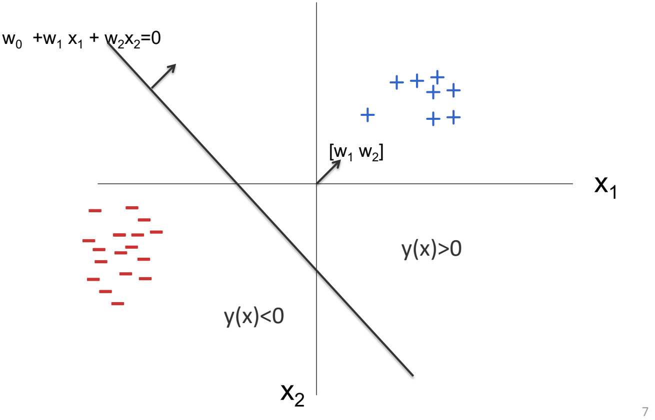
Now, it remains to "learn" the weights/parameters.

The Geometry of Linear Threshold Units

- In 2-d space, $y(\mathbf{x}) = \operatorname{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) + w_0\right)$ defines a line that separates the space.



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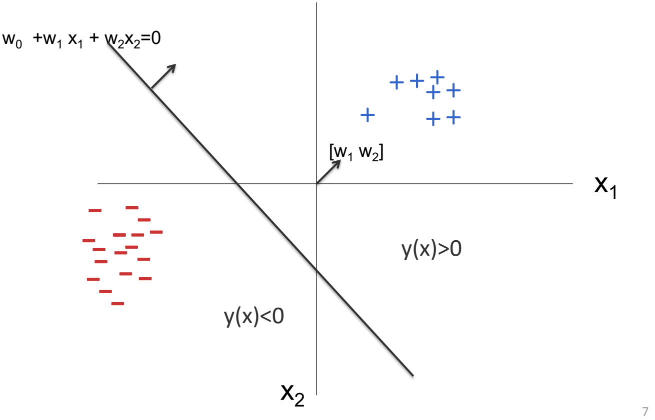

- In higher dimensional space, this corresponds to a hyperplane.

The Perceptron

REPORT NO. 85-460-1

THE PERCEPTRON

A PERCEIVING AND RECOGNIZING AUTOMATON

(PROJECT PARA)

January, 1957

Prepared by: Frank Rosenblatt

Frank Rosenblatt,
Project Engineer

Psychological Review
Vol. 65, No. 6, 1958

THE PERCEPTRON: A PROBABILISTIC MODEL FOR INFORMATION STORAGE AND ORGANIZATION IN THE BRAIN [1]

F. ROSENBLATT

Cornell Aeronautical Laboratory

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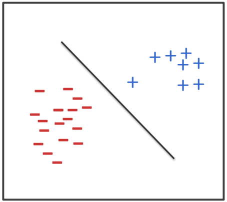
Assumptions

- Binary Classification, where $y \in \{-1, +1\}$.
- Data is **linearly separable**.



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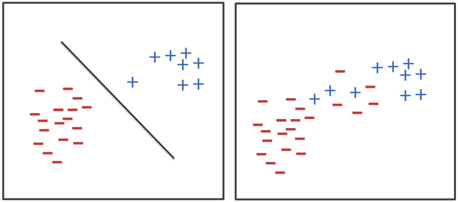

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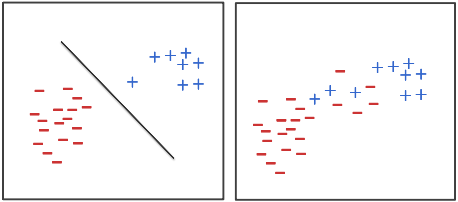

- Dummy variable:

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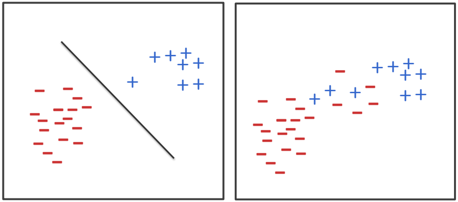

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$$y(\mathbf{x}) = \text{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) + w_0\right) \Leftrightarrow y(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \mathbf{x}).$$

Note that we abuse the notation of $\mathbf{x}$ a little bit here.

The Perceptron Algorithm

1. Initialize $\mathbf{w} = 0$
2. For each training sample $(\mathbf{x}_i, y_i) \in \mathcal{D}$:
   - If $y_i \neq \text{sign}(\mathbf{w}^\top \mathbf{x}_i)$: `# The sample is mis-classified`
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- Similar reasoning for negative samples

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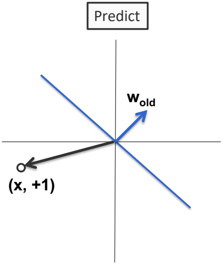

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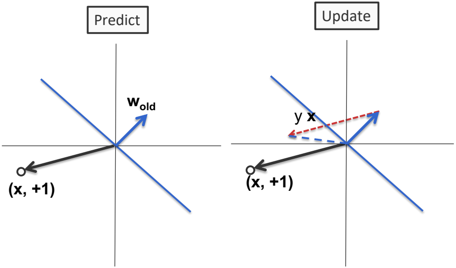

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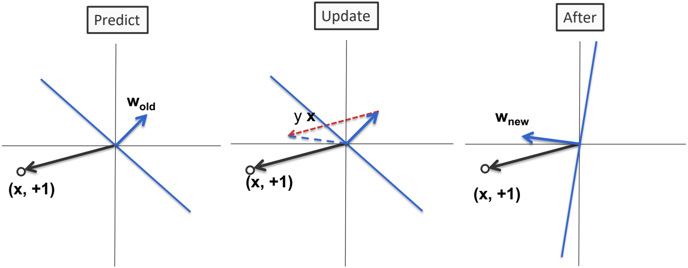

Update for a mis-classified positive sample

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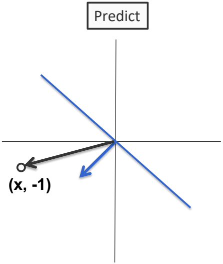

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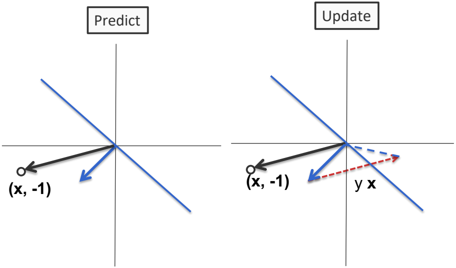

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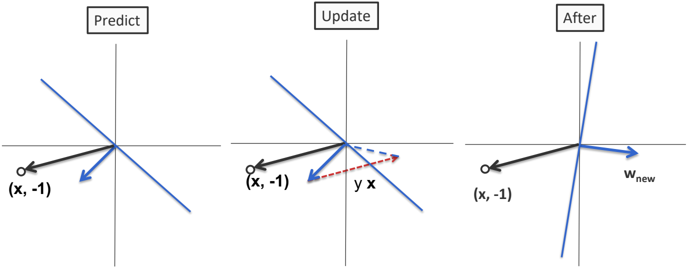

Update for a mis-classified negative sample

Theory

- If the training data is **linear separable**, then after some finite number of steps, the Perceptron algorithm will find a linear separator.
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- If the training data is **not linearly separable**, then the learning algorithm will eventually repeat the same set of weights and enter an infinite loop

Section 3

Logistic Regression

Predicting a Probability

Will someone have a heart attack over the next year?

age	62 years
gender	male
blood suger	120 mg/DL40,000
HDL	50
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blood suger	120 mg/DL40,000
HDL	50
LDL	120
Mass	190 lbs
Height	5' 10"
...	...

- Binary Classification: Two classes, i.e, $K = 2$
- For convenience, instead of $y \in \{0, 1\}$, sometimes, we use $y \in \{-1, +1\}$ to denote the two classes.
- In addition to Yes/No, we also care about the probability of heart attack : $p(y|x)$.

Generative Model Vs. Discriminative Model

- Probabilistic Generative Model
  Model the class-conditional densities $p(\mathbf{x}|y=k)$ and prior probabilities $p(y=k)$, and compute $p(y=k|\mathbf{x})$ using Bayes' theorem

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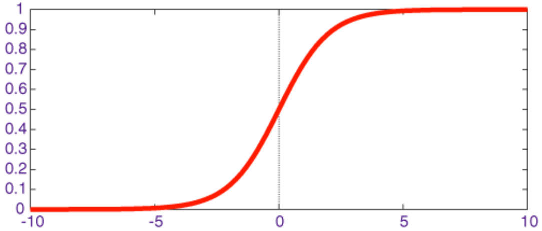
- Probabilistic Discriminative Model
  Maximize a likelihood function defined through the conditional distribution $p(y=k|\mathbf{x})$
  - Logistic Regression:

$$p(y=1|\mathbf{x}) = h(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} w_i x_i\right) = \sigma(\mathbf{w}^T\mathbf{x}).$$

Sigmoid Function σ

Logistic regression, $h(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} w_i x_i\right) = \sigma(\mathbf{w}^T\mathbf{x})$.

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



How is $\sigma(-s)$ related to $\sigma(s)$?

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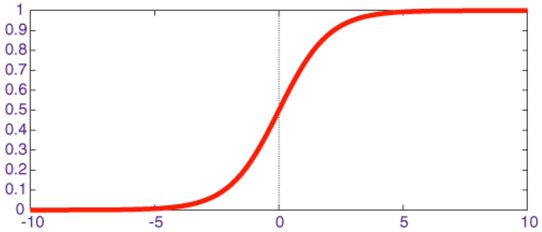

$$\sigma(-s) = \frac{e^{-s}}{1+e^{-s}} = \frac{1}{1+e^s} = 1 - \sigma(s)$$

What Makes an h Good?

$$p(y=1|\mathbf{x}) = h(\mathbf{x}) = \sigma\left(\sum_{i=0}^{d} w_i x_i\right) = \sigma(\mathbf{w}^T\mathbf{x}).$$

$$h \text{ is good if: } \begin{cases} h(\mathbf{x}_n) = \sigma(\mathbf{w}^T\mathbf{x}_n) \approx 1 & \text{whenever } y_n = +1; \\ h(\mathbf{x}_n) = \sigma(\mathbf{w}^T\mathbf{x}_n) \approx 0 & \text{whenever } y_n = -1. \end{cases}$$

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A simple error measure that captures this:

$$E(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(h(\mathbf{x}_n) - \frac{1}{2}(1+y_n)\right)^2.$$

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Hard to minimize! (The loss function is not guaranteed to be convex).

The Logistic Loss Function

$$E(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln(1 + \exp\left(-y_n \cdot \mathbf{w}^T\mathbf{x}\right))$$

It looks complicated and ugly $(\ln, e^{(\cdot)}, \dots)$,
But,

- it is based on an intuitive probabilistic interpretation of h.
- it is very convenient and mathematically friendly ('easy' to minimize).

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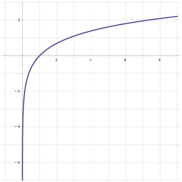
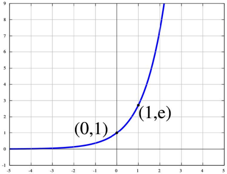
ln



exp



- For $y_n = +1$, minimizing $E(\mathbf{w})$ encourages $\mathbf{w}^T\mathbf{x}_n \gg 0$, so $h(\mathbf{x}_n) = \sigma(\mathbf{w}^T\mathbf{x}_n) \approx 1$
- For $y_n = -1$, minimizing $E(\mathbf{w})$ encourages $\mathbf{w}^T\mathbf{x}_n \ll 0$, so $h(\mathbf{x}_n) = \sigma(\mathbf{w}^T\mathbf{x}_n) \approx 0$

The Probabilistic Interpretation

Recall that we model $p(y=+1|\mathbf{x}) = h(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x})$,

$$P(y|\mathbf{x}) = \begin{cases} \sigma(\mathbf{w}^T\mathbf{x}) & \text{for } y=+1; \\ 1-\sigma(\mathbf{w}^T\mathbf{x}) & \text{for } y=-1. \end{cases}$$

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... or, more compactly

$$P(y|\mathbf{x}) = \sigma(y \cdot \mathbf{w}^T\mathbf{x})$$

The Likelihood

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Assume: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$ are independently generated.
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The probability of getting the $y_1, \ldots, y_N$ in $\mathcal{D}$ from the corresponding $\mathbf{x}_1, \ldots, \mathbf{x}_N$:

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Maximizing the Likelihood

$$
\begin{aligned}
& \max \prod_{n=1}^{N} P(y_n|\mathbf{x}_n) \\
\Leftrightarrow & \max \ln \left(\prod_{n=1}^{N} P(y_n|\mathbf{x}_n) \right) \equiv \max \sum_{n=1}^{N} \ln P(y_n|\mathbf{x}_n) \\
\Leftrightarrow & \min -\frac{1}{N} \sum_{n=1}^{N} \ln P(y_n|\mathbf{x}_n) \equiv \min \frac{1}{N} \sum_{n=1}^{N} \ln \frac{1}{P(y_n|\mathbf{x}_n)} \\
\equiv & \min \frac{1}{N} \sum_{n=1}^{N} \ln \frac{1}{\sigma(y_n \mathbf{w}^T \mathbf{x}_n)} \\
\equiv & \min \frac{1}{N} \sum_{n=1}^{N} \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n))
\end{aligned}
$$

Learning by Gradient Descent

- The gradient descent algorithm can be applied to minimize any *smooth* function, e.g.,
  - logistic regression $E(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln(1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n))$
  - ridge regression $E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} (\mathbf{w}^T \mathbf{x}_n - y_n)^2 + \lambda \|\mathbf{w}\|_2^2$

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Newton
Gradient Descent
Stocasthc gradient descent

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- When the objective function is convex, we can obtain **one** global optimal solution.
- What if the data points cannot be loaded into the memory?

Stochastic Gradient Descent (SGD)

$$E(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln(1+\exp(-y_n \cdot \mathbf{w}^T\mathbf{x}_n)) = \frac{1}{N}\sum_{n=1}^{N} \ell(\mathbf{w}, \mathbf{x}_n, y_n)$$

- A variation of GD that considers only the error on one data point.
  - Pick a random data point $(\mathbf{x}_*, y_*)$
  - Run an iteration of GD on $\ell(\mathbf{w}, \mathbf{x}_*, y_*)$

SGD for Logistic Regression

- Gradient of $\ell(\mathbf{w}, \mathbf{x}_*, y_*)$:

$$\nabla \ell(\mathbf{w}, \mathbf{x}_*, y_*) = -y_* \mathbf{x}_* \frac{\exp\left(-y_* \mathbf{w}^T \mathbf{x}_*\right)}{1 + \exp\left(-y_* \mathbf{w}^T \mathbf{x}_*\right)} = -y_* \mathbf{x}_* \frac{1}{1 + \exp\left(+y_* \mathbf{w}^T \mathbf{x}_*\right)}$$

- The update rule

$$\mathbf{w} \leftarrow \mathbf{w} + y_* \mathbf{x}_* \left(\frac{\eta}{1 + \exp\left(+y_* \mathbf{w}^T \mathbf{x}_*\right)} \right)$$

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$$\mathbf{w} \leftarrow \mathbf{w} + y_* \mathbf{x}_* \left(\frac{\eta}{1 + \exp\left(+y_* \mathbf{w}^T \mathbf{x}_*\right)} \right)$$

Recall the update of Perceptron: $\mathbf{w} \leftarrow \mathbf{w} + y_* \mathbf{x}_*$

Decision Boundary of Logistic Regression

Inference: Given an unseen data $\mathbf{x}_u$, how do the learned logistic regression model assign a label to it?

- Calculate $p(y_u = +1|\mathbf{x}_u)$ and $p(y_u = -1|\mathbf{x}_u)$

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$$\sigma(\mathbf{w}^\top \mathbf{x}) = \sigma(-\mathbf{w}^\top \mathbf{x}) \Leftrightarrow \mathbf{w}^\top \mathbf{x} = 0$$

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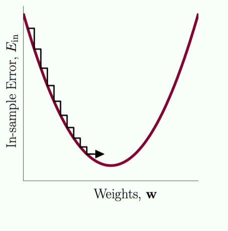
- The boundary is linear

Some Additional Notes on Step Size

η too small



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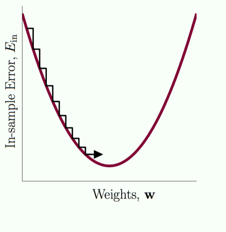

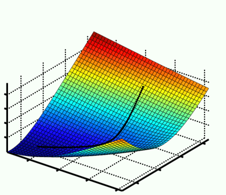

$\eta = 0.1$; 75 steps

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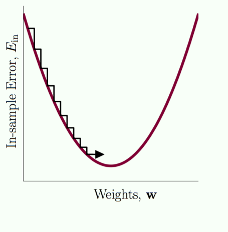

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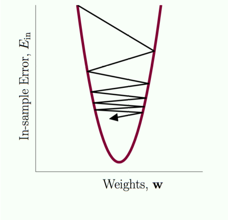

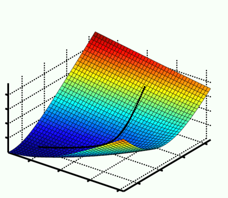

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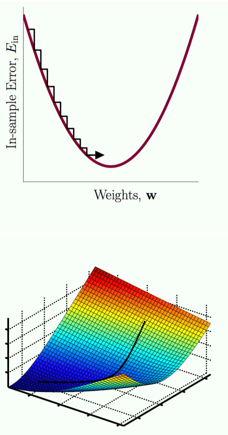

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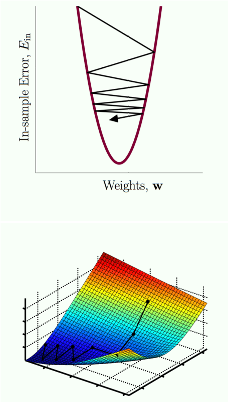

$\eta = 2$; 10 steps

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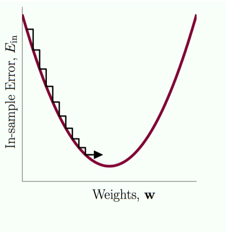

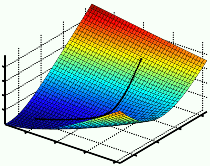

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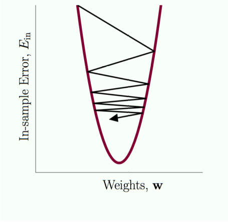
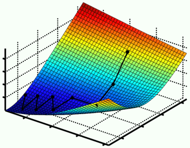
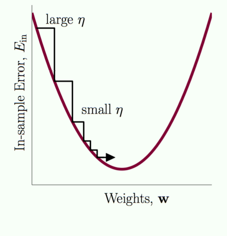




$\eta = 2$; 10 steps

η just right



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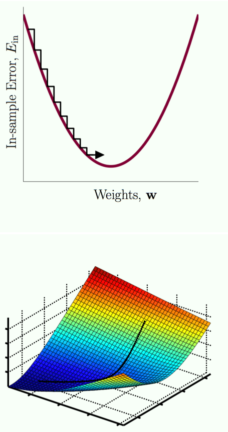

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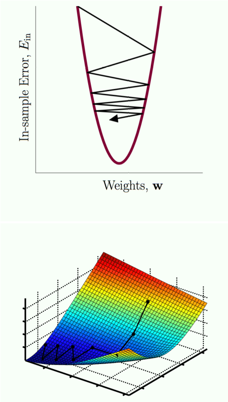

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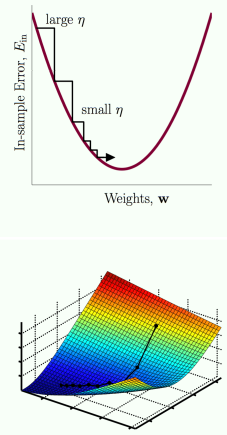

variable η_t; 10 steps