Introducción al aprendizaje automático

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#3. Funciones de costo y optimización. Árboles de decisión

Regresión polinomial

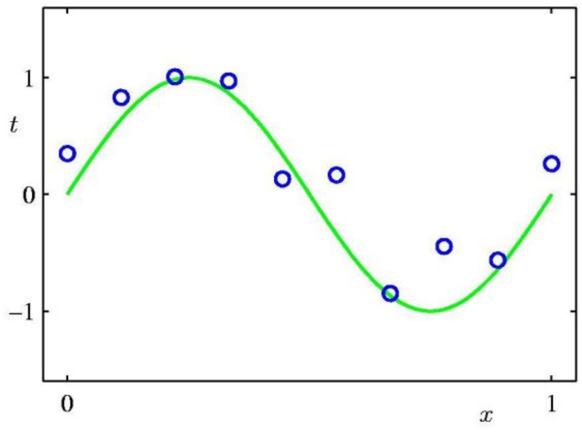
- En verde se ilustra la función "verdadera" (inaccesible)

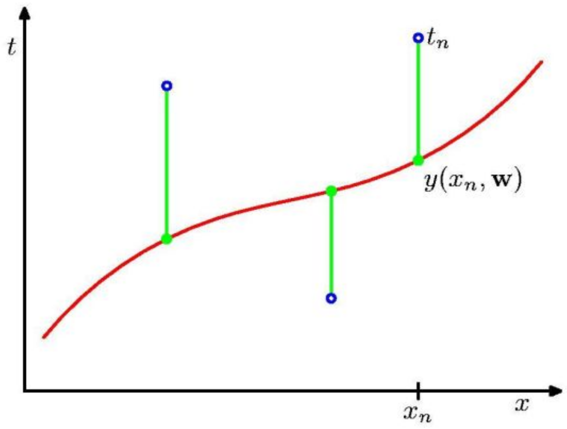
- Las muestras son uniformes en x y poseen ruido en y

- Utilizaremos una **<u>función de costo</u>** (error cuadrático) que mida el error en la predicción de y mediante $y(x,\mathrm{w})$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2$$

$$y(x,\mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$





Regresión polinomial

- Función de predicción: $y(x;w) = \sum_{j=0}^{M} w_j x^j = w^T \tilde{x}, \quad \tilde{x} = (1, x, \ldots, x^M)^T$
- Función de costo: $L(w) = \frac{1}{2} \sum_{n=0}^{N} [y_n - y(x;w)]^2$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \quad \mathbf{X} = \begin{bmatrix} \tilde{x}_1^T \\ \vdots \\ \tilde{x}_N^T \end{bmatrix} \in \mathbb{R}^{N\times(M+1)}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ \vdots \\ w_M \end{bmatrix} \in \mathbb{R}^{(M+1)}$$

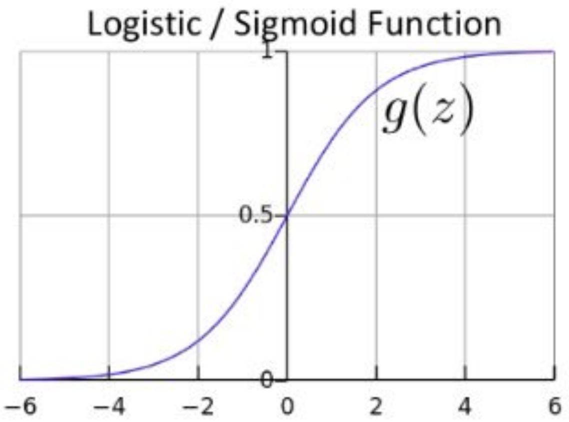
$$L(w) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) \quad \Rightarrow \quad \mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

$$L(w) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) + \lambda\mathbf{w}^T\mathbf{w} \quad \Rightarrow \quad \mathbf{w}^* = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Petersen & Pedersen, The matrix cookbook (2012)

Regresión logística

- Dados $\{(x_1, y_1), \ldots, (x_N, y_N)\}$, con $x_i \epsilon \mathbb{R}^n$, $y_i \epsilon \{0, 1\}$



- Modelo: $p(y=1|x)=h_w(x)$

$$h_w(x) = \frac{1}{1 + exp(-w^T x))}$$

- Función de costo

$$L(w) = -\sum_{i=1}^{N} y_i \log\left(h_w(x_i)\right) + (1 - y_i)\log\left(1 - h_w(x_i)\right)$$

- $h_w(x)$ no lineal → <u>no admite solución en forma cerrada</u>

Optimización y aprendizaje

- Un problema típico en ML se puede escribir como:

$$L(w) = \sum_{i=1}^{N} \ell(y_i, f_w(x_i)) + \lambda R(w)$$

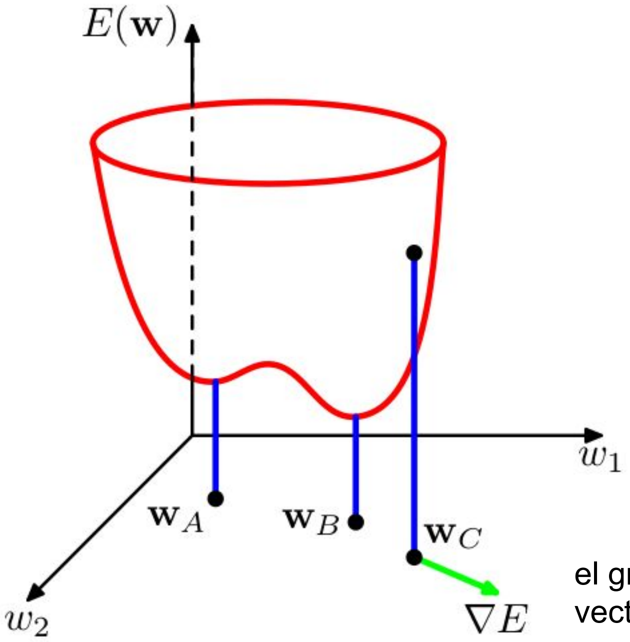
costo de predicción del par (x_i, y_i) regularización

- "Aprender" significa resolver:

$$w^* = \arg\min_w L(w)$$

... aún cuando no existan soluciones en forma cerrada.

Optimización



el gradiente de E(w) evaluado en w_C es un vector que apunta en la dirección de máximo crecimiento de la función si me paro en w_C.

- ¿La solución es única?
- Empleando algoritmos iterativos, ¿la solución depende del punto de inicio?

Funciones y conjuntos convexos

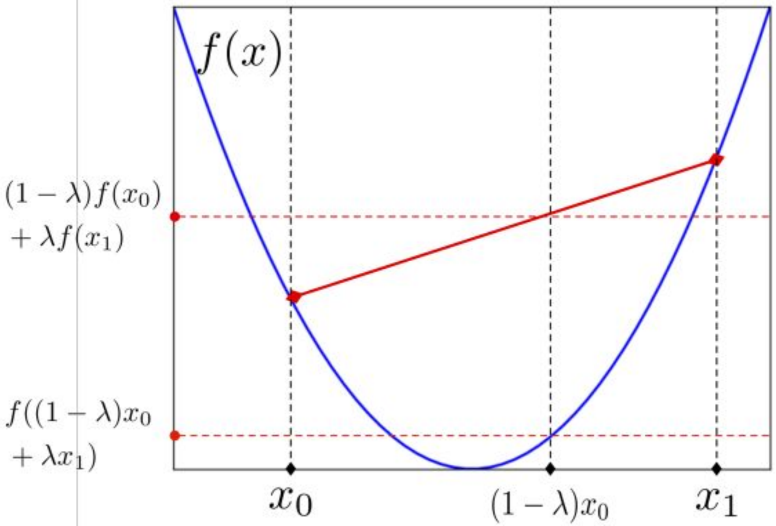
- Una **función** f es **convexa** si para cualquier x_0, x_1 en el dominio de f,

$$f((1-\lambda)x_0 + \lambda x_1) \leq (1-\lambda)f(x_0) + \lambda f(x_1), \quad 0 \leq \lambda \leq 1$$

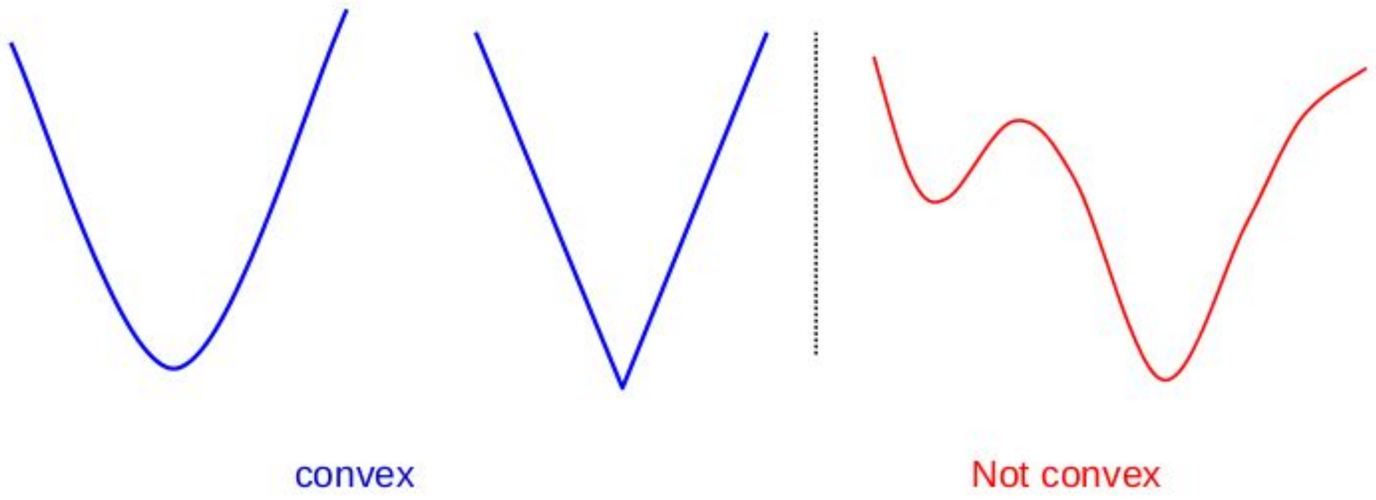
- Un **conjunto** S es **convexo** si para cualquier x_0, x_1 en S,

$$(1-\lambda)x_0 + \lambda x_1 \in S$$

- Intuitivamente la función tiene forma de "cuenco"



Ejemplo de funciones convexas



La suma no negativa de funciones convexas es convexa

Ejemplo de funciones convexas

SVM

$$\min_{\mathbf{w}\in\mathbb{R}^d} C\sum_{i}^{N} \max\left(0, 1 - y_i f(\mathbf{x}_i)\right) + ||\mathbf{w}||^2$$

convex

Porque es importante?

- Los puntos críticos (derivada=0) son todos mínimos
- Descenso de gradiente encuentra la solución óptima

Descent Methods

- The typical strategy for optimization problems of this sort is a descent method:

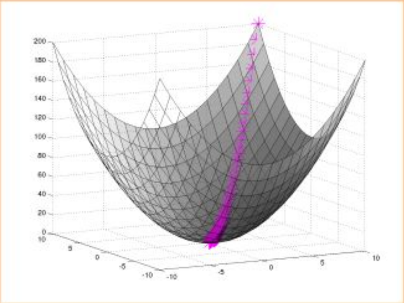
$$\boldsymbol{w}^{(\tau+1)} = \boldsymbol{w}^{(\tau)} + \Delta\boldsymbol{w}^{(\tau)}$$

- These come in many flavours
  - Gradient descent $\nabla E(\boldsymbol{w}^{(\tau)})$
  - Stochastic gradient descent $\nabla E_n(\boldsymbol{w}^{(\tau)})$
  - Newton-Raphson (second order) ∇^2

Descenso de gradiente

Algorithm 1 Gradient Descent

procedure GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
    while not converged **do**
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
    return $\boldsymbol{\theta}$



In order to apply GD to Logistic Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_N} J(\boldsymbol{\theta}) \end{bmatrix}$$

Gradiente en regresión logística

$$\log P(Y=y|X=\mathbf{x},\mathbf{w}) = \begin{cases} \log p & \text{if } y=1 \\ \log(1-p) & \text{if } y=0 \end{cases}$$

$$p \equiv \frac{1}{1+e^{-\mathbf{x}\cdot\mathbf{w}}} = \frac{1}{1+\exp(-\sum_j x^j w^j)}$$

We're going to dive into this thing here: d/dw(p)

$$(\log f)' = \frac{1}{f} f'$$

$$\frac{\partial}{\partial w^j} \log P(Y=y|X=\mathbf{x},\mathbf{w}) = \begin{cases} \frac{1}{p} \boxed{\frac{\partial}{\partial w^j} p} & \text{if } y=1 \\ \frac{1}{1-p}\left(-\frac{\partial}{\partial w^j} p\right) & \text{if } y=0 \end{cases}$$

Gradiente en regresión logística

$$\boxed{\frac{\partial}{\partial w^j} p} = \frac{\partial}{\partial w^j}(1 + \exp(-\sum_j x^j w^j))^{-1}$$

$$(f^n)' = nf^{n-1} \cdot f'$$

$$(e^f)' = e^f f'$$

$$= (-1)(1 + \exp(-\sum_j x^j w^j))^{-2} \frac{\partial}{\partial w^j} \exp(-\sum_j x^j w^j)$$

$$= (-1)(1 + \exp(-\sum_j x^j w^j))^{-2} \exp(-\sum_j x^j w^j)(-x^j)$$

$$= \underbrace{\boxed{\frac{1}{1 + \exp(-\sum_j x^j w^j)}}}_{p} \underbrace{\boxed{\frac{\exp(-\sum_j x^j w^j)}{1 + \exp(-\sum_j x^j w^j)}}}_{1-p} x^j$$

$$\frac{\partial}{\partial w^j} p = p(1-p)x^j$$

Gradiente en regresión logística

$$\frac{\partial}{\partial w^j}\log P(Y=y|X=\mathbf{x},\mathbf{w})=\begin{cases}\cancel{\frac{1}{p}}\cancel{p}(1-p)x^j=(1-p)x^j & \text{if } y=1\\ \cancel{\frac{1}{1-p}}(-1)p\cancel{(1-p)}x^j=-px^j & \text{if } y=0\end{cases}$$

$$\frac{\partial}{\partial w^j}\log P(Y=y|X=\mathbf{x},\mathbf{w})=(y-p)x^j$$

- Regla de actualización en regresión logística:

$$\mathbf{w}^{(t+1)}=\mathbf{w}^{(t)}+\lambda(y-p)\mathbf{x}$$

Details: Picking learning rate

- Use grid-search in log-space over small values on a tuning set:
  - e.g., 0.01, 0.001, …
- Sometimes, decrease after each pass:
  - e.g factor of $1/(1 + dt)$, t=epoch
  - sometimes $1/t^2$
- Fancier techniques I won't talk about:
  - Adaptive gradient: scale gradient differently for each dimension (Adagrad, ADAM, ….)

The Machine Learners Job

(1) Get the labeled data: $(x^1, y^1), \ldots, (x^n, y^n)$

(2) Choose a parametrization for hypothesis: $h_w(x)$

(3) Choose a loss function: $\ell(h_w(x), y) \geq 0$

(4) Solve the *training problem*:

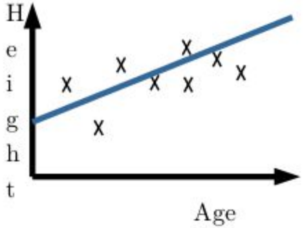
$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

(5) Test and cross-validate. If fail, go back a few steps

Parametrizing the Hypothesis

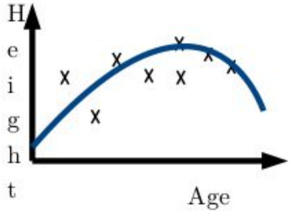
Linear:

$$h_w(x) = \sum_{i=0}^{d} w_i x_i$$

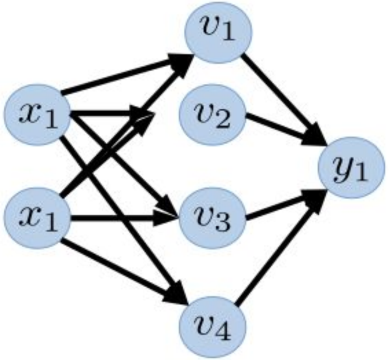


Polinomial:

$$h_w(x) = \sum_{i,j=0}^{d} w_{ij} x_i x_j$$



Neural Net:



$exe:$

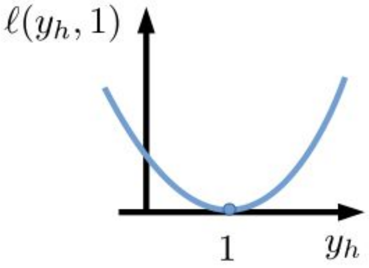
$$v_1 = \text{sign}(w_{11}x_1 + w_{12}x_2)$$

$$v_4 = 1/\left(1 + \exp(w_{41}x_1 + w_{42}x_2)\right)$$

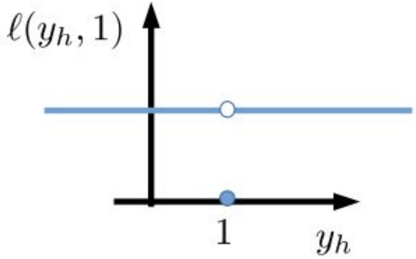
Choosing the Loss Function

Let $y_h := h_w(x)$

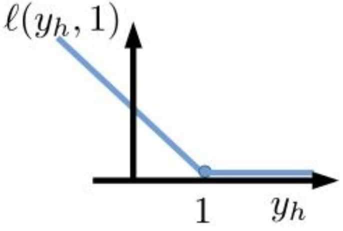
Quadratic Loss $\quad \ell(y_h, y) = (y_h - y)^2$



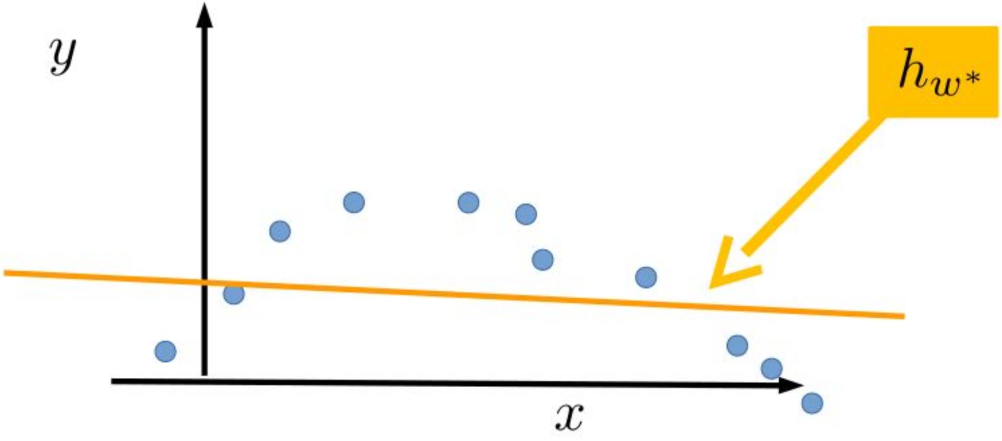
Binary Loss $\quad \ell(y_h, y) = \begin{cases} 0 & \text{if } y_h = y \\ 1 & \text{if } y_h \neq y \end{cases}$



Hinge Loss $\quad \ell(y_h, y) = \max\{0, 1 - y_h y\}$



Overfitting and Model Complexity

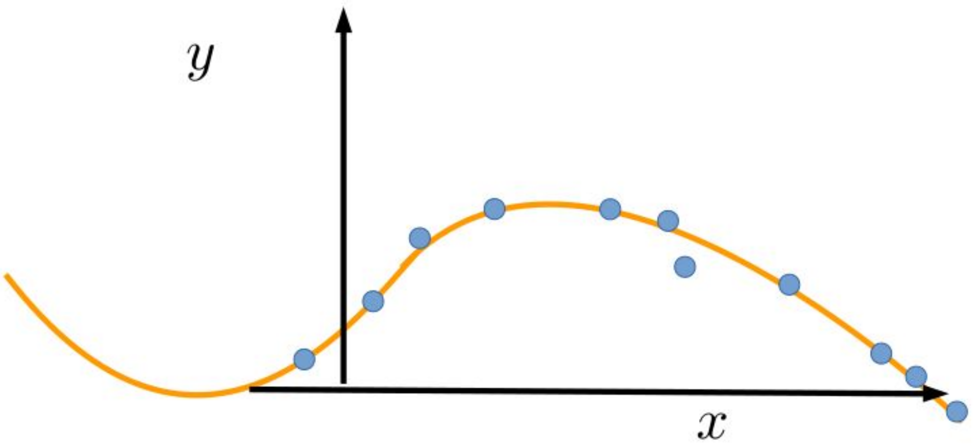


Fitting 1st order polynomial

$$h_w = \langle w, x \rangle$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i\right)^2$$

Overfitting and Model Complexity

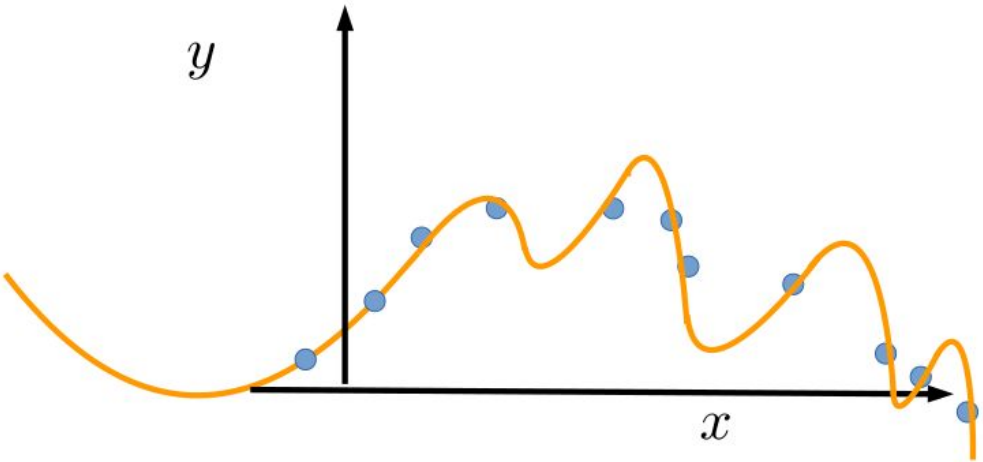


Fitting 3rd order polynomial

$$h_w = \sum_{i=0}^{3} w_i x^i$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i\right)^2$$

Overfitting and Model Complexity



Fitting 9th order polynomial

$$h_w = \sum_{i=0}^{9} w_i x^i$$

$$w^* = \arg\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left(h_w(x^i) - y^i\right)^2$$

Regularization

Regularizor Functions

$$
\begin{aligned}
R: \quad \mathbf{R}^d &\rightarrow \mathbf{R}_+ \\
w &\rightarrow R(w)
\end{aligned}
$$

Controls tradeoff between fit and complexity

General Training Problem

$$
\min_{w \in \mathbf{R}^d} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right)}_{\text{Goodness of fit, fidelity term ...etc}} + \underbrace{\lambda R(w)}_{\text{Penlizes complexity}}
$$

Goodness of fit, fidelity term ...etc

Penlizes complexity

Exe: Ridge Regression

Linear hypothesis

$$h_w(x) = \langle w, x \rangle$$

L2 regularizor

$$R(w) = ||w||_2^2$$

L2 loss

$$\ell(y_h, y) = (y_h - y)^2$$

Ridge Regression

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} (y^i - \langle w, x^i \rangle)^2 + \lambda ||w||_2^2$$

Exe: Logistic Regression

Linear hypothesis

$$h_w(x) = \langle w, x \rangle$$

+

L2 regularizor

$$R(w) = ||w||_2^2$$

Logistic loss

$$\ell(y_h, y) = \ln(1 + e^{-y y_h})$$

$(y \in \{-1, +1\})$

Logistic Regression

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ln(1 + e^{-y^i \langle w, x^i \rangle}) + \lambda ||w||_2^2$$

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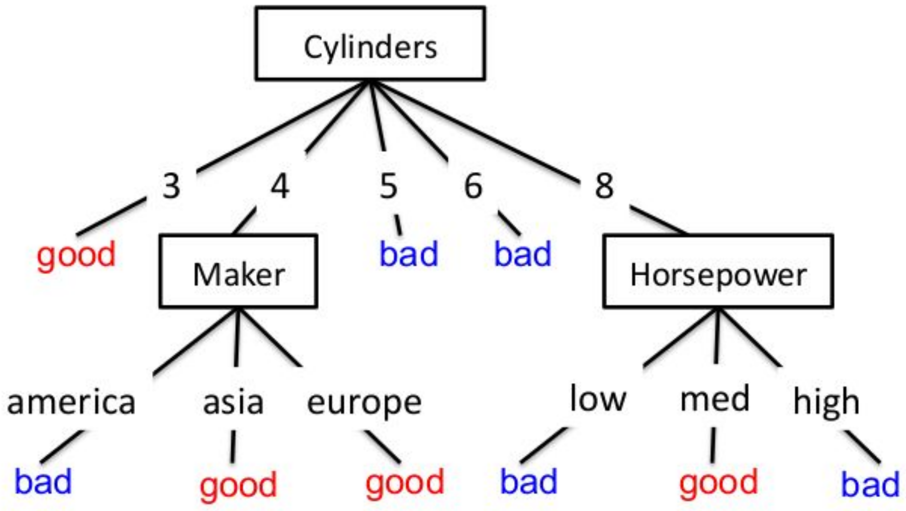
Árboles de decisión

Hypotheses: decision trees $f : X \rightarrow Y$

- Each internal node tests an attribute x_i
- One branch for each possible attribute value $x_i = v$
- Each leaf assigns a class y
- To classify input x: traverse the tree from root to leaf, output the labeled y

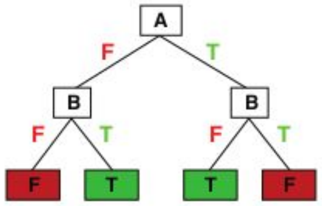


Human interpretable!

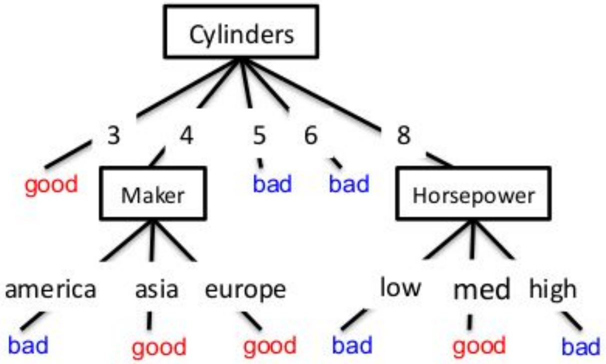
What functions can be represented?

- Decision trees can represent any function of the input attributes!
- For Boolean functions, path to leaf gives truth table row
- Could require exponentially many nodes

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



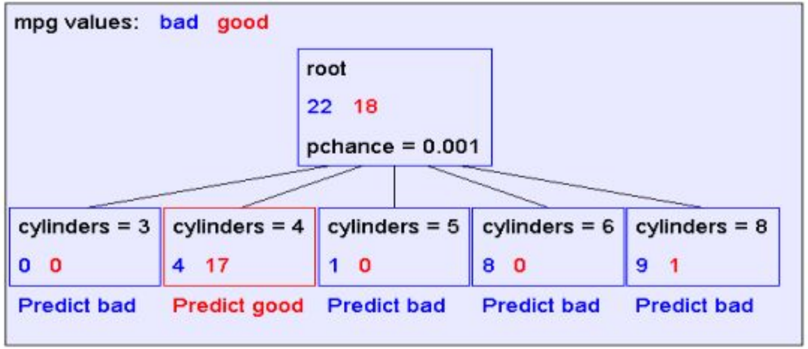
(Figure from Stuart Russell)

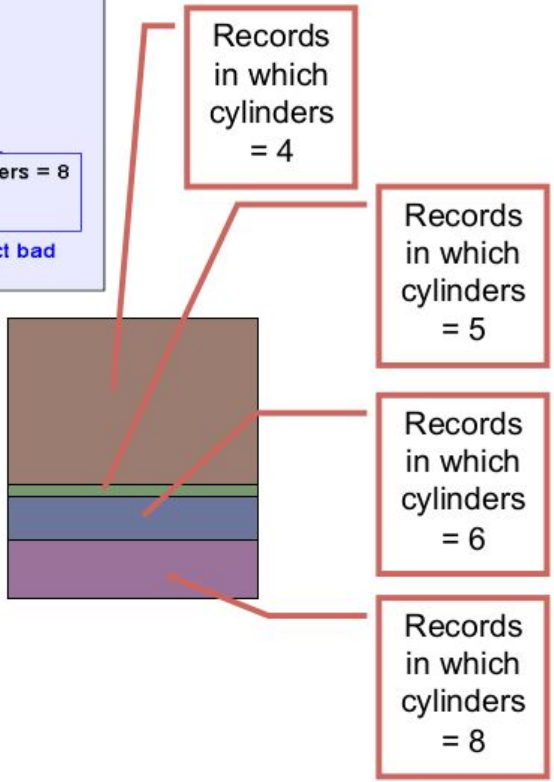


Learning *simplest* decision tree is NP-hard

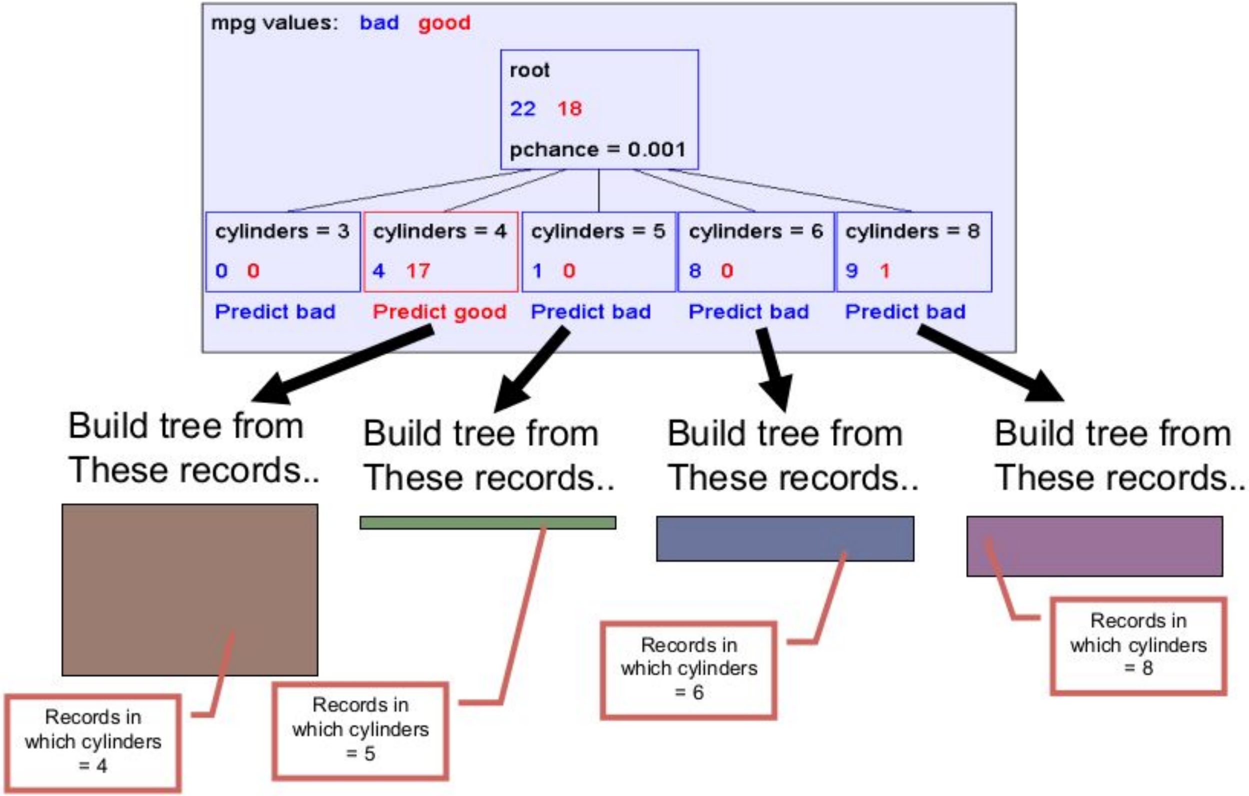
- Learning the simplest (smallest) decision tree is an NP-complete problem [Hyafil & Rivest '76]
- Resort to a greedy heuristic:
  - Start from empty decision tree
  - Split on **next best attribute (feature)**
  - Recurse

Key idea: Greedily learn trees using **recursion**





Recursive Step



Splitting: choosing a good attribute

Would we prefer to split on X_1 or X_2?

Idea: use counts at leaves to define probability distributions, so we can measure uncertainty!

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F
F	T	F
F	F	F

Measuring uncertainty

- Good split if we are more certain about classification after split
  - Deterministic good (all true or all false)
  - Uniform distribution bad
  - What about distributions in between?

P(Y=A) = 1/2	P(Y=B) = 1/4	P(Y=C) = 1/8	P(Y=D) = 1/8

P(Y=A) = 1/4	P(Y=B) = 1/4	P(Y=C) = 1/4	P(Y=D) = 1/4

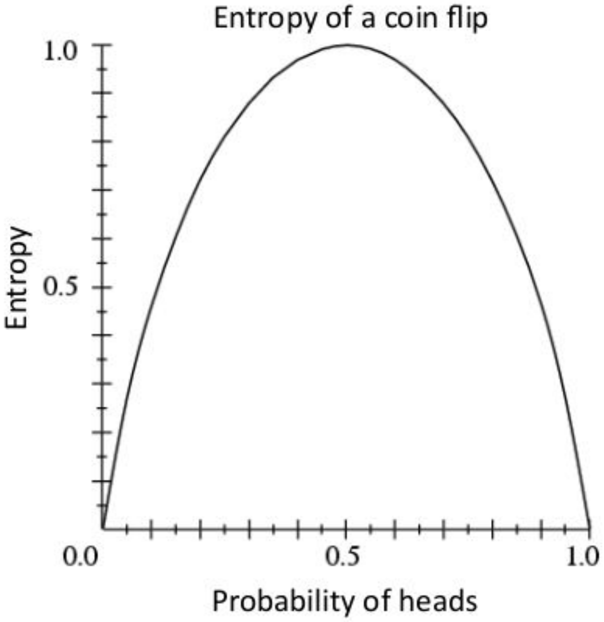
Entropy

Entropy $H(Y)$ of a random variable Y

$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

More uncertainty, more entropy!

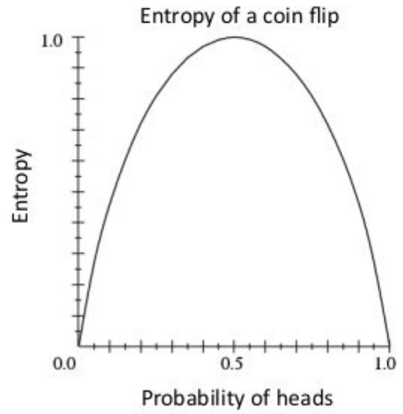
Information Theory interpretation:
$H(Y)$ is the expected number of bits needed to encode a randomly drawn value of Y (under most efficient code)



High, Low Entropy

- "High Entropy"
  - Y is from a uniform like distribution
  - Flat histogram
  - Values sampled from it are less predictable
- "Low Entropy"
  - Y is from a varied (peaks and valleys) distribution
  - Histogram has many lows and highs
  - Values sampled from it are more predictable

Entropy Example



$$H(Y) = -\sum_{i=1}^{k} P(Y = y_i) \log_2 P(Y = y_i)$$

P(Y=t) = 5/6

P(Y=f) = 1/6

H(Y) = - 5/6 $\log_2$ 5/6 - 1/6 $\log_2$ 1/6

= 0.65

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

Conditional Entropy

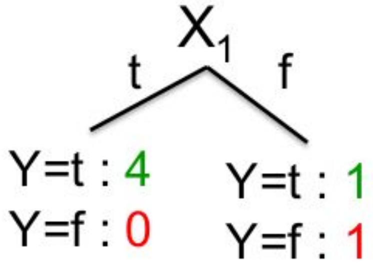
Conditional Entropy $H(Y|X)$ of a random variable Y conditioned on a random variable X

$$H(Y \mid X) = -\sum_{j=1}^{v} P(X = x_j) \sum_{i=1}^{k} P(Y = y_i \mid X = x_j) \log_2 P(Y = y_i \mid X = x_j)$$

Example:

$P(X_1=t) = 4/6$

$P(X_1=f) = 2/6$



X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

$H(Y|X_1) = -\ 4/6\ (1 \log_2 1 + 0 \log_2 0)$

$\quad -\ 2/6\ (1/2 \log_2 1/2 + 1/2 \log_2 1/2)$

$= 2/6$

Information gain

- Decrease in entropy (uncertainty) after splitting

$$IG(X) = H(Y) - H(Y \mid X)$$

In our running example:

$IG(X_1) = H(Y) - H(Y|X_1)$
$= 0.65 - 0.33$

$IG(X_1) > 0 \rightarrow$ we prefer the split!

X_1	X_2	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F

Learning decision trees

- Start from empty decision tree
- Split on **next best attribute (feature)**
  - Use, for example, information gain to select attribute:

$$\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$$

- Recurse

Decision trees will overfit

- Standard decision trees have no learning bias
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Must introduce some bias towards simpler trees
- Many strategies for picking simpler trees
  - Fixed depth
  - Minimum number of samples per leaf
- Random forests

Real-Valued inputs

What should we do if some of the inputs are real-valued?

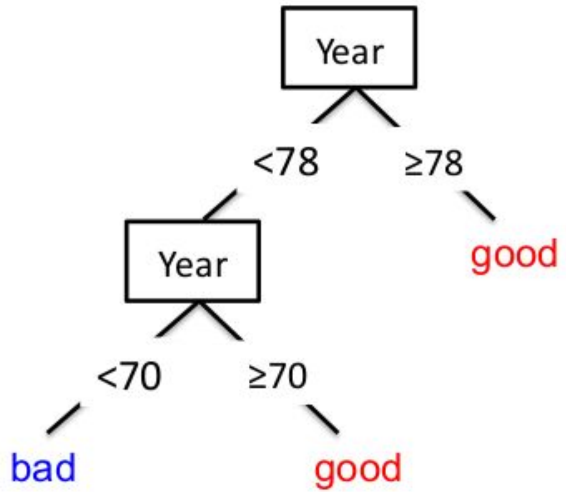
Infinite number of possible split values!!!

mpg	cylinders	displacemen	horsepower	weight	acceleration	modelyear	maker
good	4	97	75	2265	18.2	77	asia
bad	6	199	90	2648	15	70	america
bad	4	121	110	2600	12.8	77	europe
bad	8	350	175	4100	13	73	america
bad	6	198	95	3102	16.5	74	america
bad	4	108	94	2379	16.5	73	asia
bad	4	113	95	2228	14	71	asia
bad	8	302	139	3570	12.8	78	america
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
good	4	120	79	2625	18.6	82	america
bad	8	455	225	4425	10	70	america
good	4	107	86	2464	15.5	76	europe
bad	5	131	103	2830	15.9	78	europe

Threshold splits

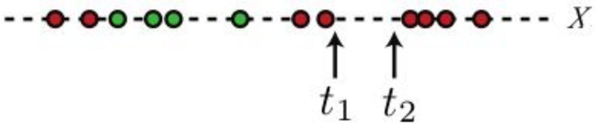
- Binary tree: split on attribute X at value t
  - One branch: X < t
  - Other branch: X ≥ t

- Requires small change
  - Allow repeated splits on same variable **along a path**

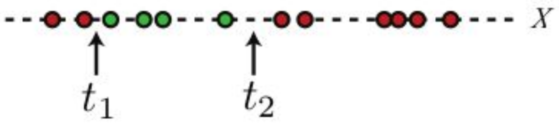


The set of possible thresholds

- Binary tree, split on attribute X
  - One branch: X < t
  - Other branch: X ≥ t
- Search through possible values of *t*
  - Seems hard!!!
- But only a finite number of *t*'s are important:



  - Sort data according to X into $\{x_1,\ldots,x_m\}$
  - Consider split points of the form $x_i + (x_{i+1} - x_i)/2$
  - Morever, only splits between examples of different classes matter!



(Figures from Stuart Russell)

Picking the best threshold

- Suppose *X* is real valued with threshold *t*
- Want **IG(Y | X:t)**, the information gain for Y when testing if *X* is greater than or less than *t*
- Define:
  - H(Y|X:t) = p(X < t) H(Y|X < t) + p(X >= t) H(Y|X >= t)
  - IG(Y|X:t) = H(Y) - H(Y|X:t)
  - IG*(Y|X) = $\max_t$ IG(Y|X:t)
- Use: IG*(Y|X) for continuous variables

What you need to know about decision trees

- Decision trees are one of the most popular ML tools
  - Easy to understand, implement, and use
  - Computationally cheap (to solve heuristically)
- Information gain to select attributes (ID3, C4.5,…)
- Presented for classification, can be used for regression and density estimation too
- Decision trees will overfit!!!
  - Must use tricks to find “simple trees”, e.g.,
    - Fixed depth/Early stopping
    - Pruning
  - Or, use ensembles of different trees (random forests)