Bayes Decision Theory - I

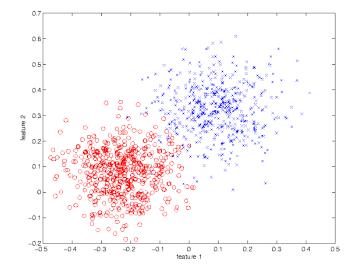
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Statistical Learning from Data

• **Goal:** Given a relationship between a feature vector *x* and a vector *y*, and iid data samples (x_i, y_i) , find an approximating function $f(x) \approx y$

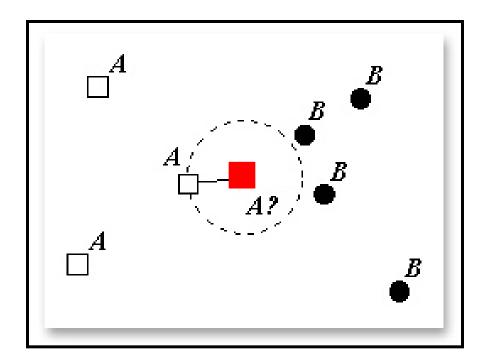
$$x \qquad \qquad \hat{y} = f(x) \approx y$$



- This is called training or learning.
- Two major types of learning:
 - Unsupervised (aka Clustering) : only X is known.
 - Supervised (Classification or Regression): both X and target value Y are known during training, only X is known at test time.

Nearest Neighbor Classifier

- The simplest possible classifier that one could think of:
 - It consists of assigning to a new, unclassified vector the same class label as that of the closest vector in the labeled training set
 - E.g. to classify the unlabeled point "Red":
 - measure Red's distance to all other labeled training points
 - If the closest point to Red is labeled "A = square", assign it to the class A
 - otherwise assign Red to the "B = circle" class



• This works a lot better than what one might expect, particularly if there are a lot of labeled training points

Nearest Neighbor Classifier

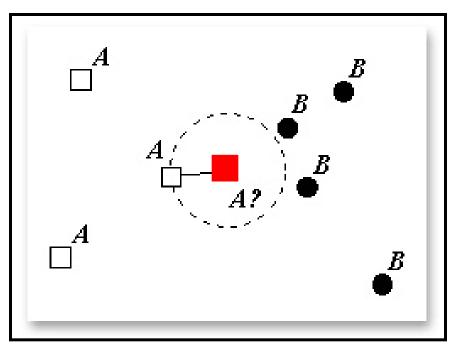
- To define this classification procedure rigorously, define:
 - a Training Set $D = \{(x_1, y_1), ..., (x_n, y_n)\}$
 - $-x_i$ is a vector of observations, y_i is the class label
 - a new vector x to classify
- The Decision Rule is

set
$$y = y_{i^*}$$

where

$$i^* = \underset{i \in \{1, \dots, n\}}{\operatorname{arg\,min}} d(x, x_i)$$

argmin means: "the *i* that minimizes the distance"



Metrics

• we have seen some examples:

- R^d

Inner Product :

$$\langle x, y \rangle = x^T y = \sum_{i=1}^d x_i y_i$$

Euclidean norm:

$$||x|| = \sqrt{x^T x} = \sqrt{\sum_{i=1}^d x_i^2}$$

Euclidean distance:

$$d(x, y) = ||x - y|| = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$$

-- Continuous functions

Inner Product :

$$\langle f(x), g(x) \rangle = \int f(x)g(x)dx$$

norm² = 'energy':
$$\|f(x)\| = \sqrt{\int f^2(x)dx}$$

Distance² = 'energy' of difference:
$$d(f,g) = \sqrt{\int [f(x) - g(x)]^2 dx}$$

Euclidean distance

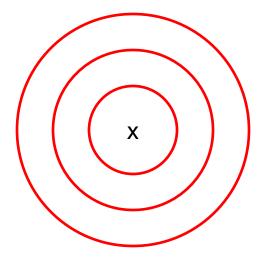
• We considered in detail the Euclidean distance

$$d(x, y) = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$$

• Equidistant points to x?

$$d(x, y) = r \Leftrightarrow \sum_{i=1}^{d} (x_i - y_i)^2 = r^2$$

- E.g.
$$(x_1 - y_1)^2 + (x_2 - y_2)^2 = r^2$$



- The equidistant points to x are on spheres around x
- Why would we need any other metric?

Inner Products

- fish example:
 - features are L = fish length, W = scale width
 - measure L in meters and W in milimeters
 - typical L: 0.70m for salmon, 0.40m for sea-bass
 - typical W: 35mm for salmon, 40mm for sea-bass
 - I have three fish
 - $F_1 = (.7,35)$ $F_2 = (.4, 40)$ $F_3 = (.75, 37.8)$
 - F₁ clearly salmon, F₂ clearly sea-bass, F₃ looks like salmon
 - yet

$$d(F_1,F_3) = 2.8 > d(F_2,F_3) = 2.23$$

- there seems to be something wrong here
- but if scale width is *also* measured in meters:
 - $F_1 = (.7, .035)$ $F_2 = (.4, .040)$ $F_3 = (.75, .0378)$
 - and now

 $d(F_1,F_3) = .05 < d(F_2,F_3) = 0.35$

- which seems to be right - the units are *commensurate*



Inner Product

- Suppose the scale width is also measured in meters:
 - I have three fish
 - $F_1 = (.7, .035)$ $F_2 = (.4, .040)$ $F_3 = (.75, .0378)$
 - and now

 $d(F_1,F_3) = .05 < d(F_2,F_3) = 0.35$

- which seems to be right
- The problem is that the Euclidean distance depends on the units (or scaling) of each axis
 - e.g. if I multiply the second coordinate by 1,000

$$d'(x, y) = \sqrt{(x_1 - y_1)^2 + 1,000,000(x_2 - y_2)^2}$$

The 2nd coordinates influence on the distance increases 1,000-fold!

• Often "right" units are not clear (e.g. car speed vs weight)

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Inner Products

- We need to work with the "right", or at least "better", units
- Apply a transformation to get a "better" feature space

$$x' = Ax$$

• examples:

- Taking A = R, R proper and orthogonal, is equivalent to a *rotation*
- Another important special case is scaling (A = S, for S diagonal)

$$\begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \lambda_1 x_1 \\ \vdots \\ \lambda_n x_n \end{bmatrix}$$

- We can combine these two transformations by making taking A = SR R

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SR

(Weighted) Inner Products

- Thus, in general one can rotate and scale by applying some matrix A = SR, to form transformed vectors x' = Ax
- What is the inner product in the new space?

$$(x')^T y' = (Ax)^T Ay = x^T \underbrace{A^T A}_M y$$

• The inner product in the new space is of weighted form in the old space

$$\langle x', y' \rangle = x^T M y$$

• Using a weighted inner product, is equivalent to working in the transformed space

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SR

(Weighted) Inner Products

- Can I use any weighting matrix M ? NO!
- Recall: an inner product is a bilinear form such that

i)
$$\langle x, x \rangle \ge 0$$
, $\forall x \in \mathcal{H}$
ii) $\langle x, x \rangle = 0$ if and only if $x = 0$
iii) $\langle x, y \rangle = \langle y, x \rangle$ for all x and y

• From iii), M must be Symmetric since

$$\langle x, y \rangle = x^T M y = (y^T M^T x)^T = y^T M^T x$$
 and
 $\langle x, y \rangle = \langle y, x \rangle = y^T M x, \quad \forall x, y$

• from i) and ii), M must be Positive Definite

$$\langle x,x\rangle = x^T M x > 0, \quad \forall x \neq 0$$

Positive Definite Matrices

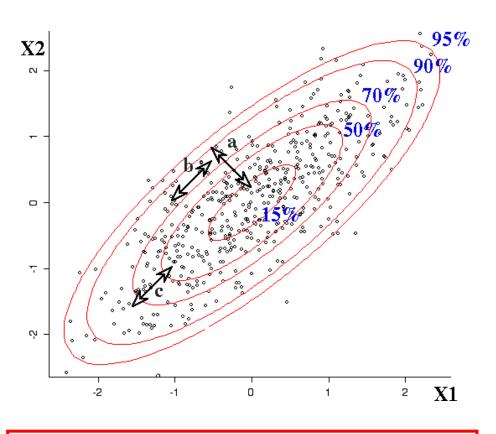
- Fact: Each of the following is a necessary and sufficient condition for a real symmetric matrix *A* to be positive definite:
 - i) $x^T A x > 0, \forall x \neq 0$
 - ii) All eigenvalues, λ_i , of A are real and satisfy $\lambda_i > 0$
 - iii) All upper-left submatrices A_k have strictly positive determinant
 - iv) There is a matrix R with independent columns such that $A = R^T R$
- Note: from property iv), we see that using a positive definite matrix A to weight an inner product is the same as working in a transformed space.
- Definition of upper left submatrices:

$$A_{1} = a_{1,1} \qquad A_{2} = \begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{bmatrix} \qquad A_{3} = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \end{bmatrix}$$

Metrics

- What is a good weighting matrix M ?
 - Let the data tell us!
 - Use the inverse of the covariance matrix $M = \sum^{-1}$

$$\Sigma = E[(x - \mu)(x - \mu)^T]$$
$$\mu = E[x]$$



• Mahalanobis Distance:

$$d(x, y) = \sqrt{(x - y)^T \Sigma^{-1} (x - y)}$$

 This distance is adapted to the covariance ("scatter") of the data and thereby provides a "natural" rotation and scaling for the data 13

The Multivariate Gaussian

- In fact, for Gaussian data, the Mahalanobis distance tells us all we could statistically know about the data
 - The pdf for a d-dimensional Gaussian of mean μ and covariance Σ is

$$P_{X}(x) = \frac{1}{\sqrt{(2\pi)^{d} |\Sigma|}} \exp\left\{-\frac{1}{2}(x-\mu)^{T}\Sigma^{-1}(x-\mu)\right\}$$

Note that this can be written as

$$P_X(x) = \frac{1}{K} \exp\left\{-\frac{1}{2}d^2(x,\mu)\right\}$$

- I.e. a Gaussian is just the exponential of the negative of the square of the Mahalanobis distance
- The constant *K* is needed only to ensure the density integrates to 1

The Multivariate Gaussian

- Using Mahalanobis = assuming Gaussian data
- Mahalanobis distance: Gaussian pdf:

$$\frac{d^{2}(x,\mu) = (x-\mu)^{T} \Sigma^{-1}(x-\mu)}{\sqrt{(2\pi)^{d} |\Sigma|}} \exp\left\{-\frac{1}{2}(x-\mu)^{T} \Sigma^{-1}(x-\mu)\right\}$$

- Points of high probability are those of small Mahalanobis distance to the center (mean) of a Gaussian density
- This can be interpreted as the right norm for a certain type of space

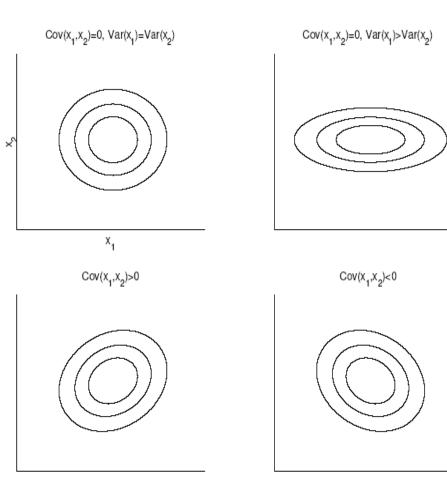
The Multivariate Gaussian

- Defined by two parameters
 - Mean just shifts center
 - Covariance controls shape

- in 2D,
$$X = (X_1, X_2)^T$$

 $\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}$

- σ_i^2 is variance of X_i
- $\sigma_{12} = cov(X_1, X_2)$ controls how dependent X_1 and X_2 are
- Note that, when $\sigma_{12} = 0$:



 $P_{X_1,X_2}(x_1,x_2) = P_{X_1}(x_1)P_{X_2}(x_2) \Leftrightarrow X_i$ are independent

The multivariate Gaussian

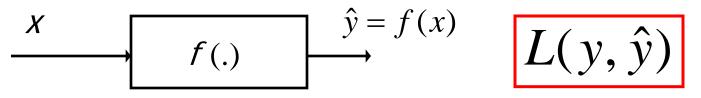
- this applet allows you to view the impact of the covariance parameters
- <u>http://www.sfu.ca/~vkyrylov/Java%20Applets/Distribution</u> <u>3D/ThreeDSurface/classes/ThreeDSurface.htm</u>
- note: they show

$$\rho = \frac{\sigma_{12}}{\sigma_1 \sigma_2}$$

• but since you do not change σ_1 and σ_2 when you are changing ρ , this has the same impact as changing σ_{12}

"Optimal" Classifiers

- Some metrics are *"better"* than others
- The meaning of "better" is connected to how well adapted the metric is to the properties of the data
- Can we be more rigorous? Can we have an "optimal" metric? What could we mean by "optimal"?
- To talk about *optimality* we start by defining *cost* or *loss*



- Cost is a real-valued loss function that we want to minimize
- It depends on the true y and the prediction \hat{y}
- The value of the cost tells us how good our predictor \hat{y} is

Loss Functions for Classification

- Classification Problem: loss is function of classification errors
 - What types of errors can we have?
 - Two Types: False Positives and False Negatives
 - Consider a face detection problem
 - If you see these two images and say





say = "non-face"

 you have a false-positive

false-negative (miss)

- Obviously, we have similar sub-classes for non-errors
 - true-positives and true-negatives
- The positive/negative part reflects what we say
- The true/false part reflects the *real classes*

Loss functions

- are some errors more important than others?
 - depends on the problem
 - consider a snake looking for lunch
 - the snake likes frogs
 - but dart frogs are highly poisonous
 - the snake must classify each frog it sees

Y = {"dart", "regular"}

- the losses are clearly different

snake prediction	Frog =dart	Frog= regular
"regular"	8	0
"dart"	0	10



Loss functions

- but not all snakes are the same
 - this one is a dart frog predator
 - it can still classify each frog it sees
 - Y = {"dart", "regular"}
 - it actually prefers dart frogs
 - but the other ones are good to eat too

snake prediction	Frog =dart	Frog= regular
"regular"	10	0
"dart"	0	10



(Conditional) Risk as Average Cost

• Given a loss function, denote the *cost* of classifying a data vector *x* generated from class *j* as *i* by

$$L[j \rightarrow i]$$

 Conditioned on an observed data vector x, to measure how good the classifier is, on average, use the (conditional) expected value of the loss, aka the (conditional) Risk,

$$R(x,i) \stackrel{\text{def}}{=} \operatorname{E}\{L[Y \to i] \mid x\} = \sum_{j} L[j \to i] P_{Y|X}(j \mid x)$$

- This means that the *risk of classifying x as i* is equal to
 - the sum, over all classes *j*, of the cost of classifying *x* as *i* when the truth is *j* times the conditional probability that the true class is *j* (where the conditioning is on the observed value of *x*)

- Note that:
 - This immediately allows us to define an optimal classifier as the one that minimizes the (conditional) risk
 - For a given observation x, the Optimal Decision is given by

$$i^{*}(x) = \arg\min_{i} R(x,i)$$

= $\arg\min_{i} \sum_{j} L[j \rightarrow i] P_{Y|X}(j \mid x)$

and it has optimal (minimal) risk given by

$$R^{*}(x) = \min_{i} R(x,i) = \min_{i} \sum_{j} L[j \to i] P_{Y|X}(j \mid x)$$

- Back to our example
 - A snake sees this



and makes probability assessments

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

and computes the optimal decision



• Info an ordinary snake is presumed to have

Class probabilities *conditioned on x*

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

Ordinary Snake Losses

snake prediction	dart frog	regular frog
"regular"	8	0
"dart"	0	10

• The risk of saying "regular" given the observation x is

$$\sum_{j} L[j \rightarrow \operatorname{reg}] P_{Y|X}(j \mid x) =$$

$$= L[\operatorname{reg} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{reg} \mid x) + L[\operatorname{dart} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{dart} \mid x)$$

$$= 0 \times 1 + \infty \times 0 = 0 + 0 = 0$$
25

• Info the ordinary snake has for the given observation x

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

snake prediction	dart frog	regular frog
"regular"	8	0
"dart"	0	10

• Risk of saying "dart" given x is

$$\sum_{j} L[j \rightarrow dart] P_{Y|X}(j \mid x) =$$

$$= L[reg \rightarrow dart] P_{Y|X}(reg \mid x) + L[dart \rightarrow dart] P_{Y|X}(dart \mid x)$$

$$= 10 \times 1 + 0 \times 0 = 10 + 0 = 10$$

Optimal decision = say *"regular"*. Snake says *"regular"* given the observation x and has a good, safe lunch ^(C) (risk = 0)

- The next time the ordinary snake goes foraging for food
 - It sees this image x



- It "knows" that dart frogs can be colorful
- So it assigns a nonzero probability to this image *x* showing a dart frog

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$



Info the ordinary snake has given the new measurement x

Class probabilities conditioned on new x

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$

Ordinary Snake Losses

snake prediction	dart frog	regular frog
"regular"	∞	0
"dart"	0	10

• The risk of saying "regular" given the new observation x is

$$\sum_{j} L[j \rightarrow \operatorname{reg}] P_{Y|X}(j \mid x) =$$

$$= L[\operatorname{reg} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{reg} \mid x) + L[\operatorname{dart} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{dart} \mid x)$$

$$= 0 \times 0.9 + \infty \times 0.1 = \infty$$
28

• Info the snake has given x

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$

• Risk of saying *"dart"* given *x* is

Ordinary Snake Losses

snake prediction	dart frog	regular frog
"regular"	8	0
"dart"	0	10

$$\sum_{j} L[j \rightarrow dart] P_{Y|X}(j \mid x) =$$

$$= L[reg \rightarrow dart] P_{Y|X}(reg \mid x) + L[dart \rightarrow dart] P_{Y|X}(dart \mid x)$$

$$= 10 \times 0.9 + 0 \times 0.1 = 9$$

- The snake decides "dart" and looks for another frog
 even though this is a regular frog with 0.9 probability
- Note that this is always the case unless $P_{Y|X}(dart|X) = 0_{29}$

- What about the "dart-snake" that can safely eat dart frogs?
 - The dart-snake sees this



and makes probability assessments

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

and computes the optimal decision



• Info the dart-snake has given x

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

Dart-Snake Losses

snake prediction	dart frog	regular frog
"regular"	10	0
"dart"	0	10

• Risk of saying *"regular" given x* is

$$\sum_{j} L[j \rightarrow \operatorname{reg}] P_{Y|X}(j \mid x) =$$

$$= L[\operatorname{reg} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{reg} \mid x) + L[\operatorname{dart} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{dart} \mid x)$$

$$= 0 \times 1 + 10 \times 0 = 0$$

• Info the dart-snake has given x

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

Dart-Snake Losses

snake prediction	dart frog	regular frog
regular	10	0
dart	0	10

• Risk of dart-snake deciding "dart" given x is

$$\sum_{j} L[j \rightarrow dart] P_{Y|X}(j \mid x) =$$

$$= L[reg \rightarrow dart] P_{Y|X}(reg \mid x) + L[dart \rightarrow dart] P_{Y|X}(dart \mid x)$$

$$= 10 \times 1 + 0 \times 0 = 10$$

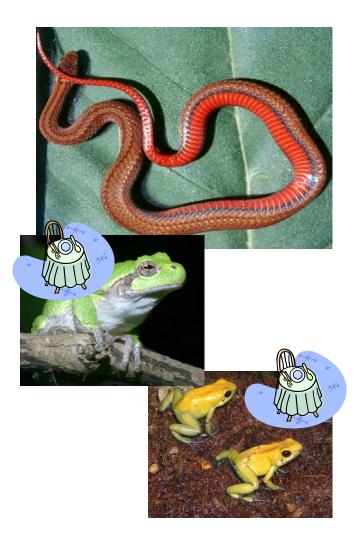
• Dart-snake optimally decides *"regular"*, which is consistent with the *x*-conditional class probabilities

• Now the dart-snake sees this



 Let's assume that it makes the same probability assignments as the ordinary snake

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$



• Info dart-snake has given new x

 $P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$

Dart-Snake L	osses
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snake prediction	dart frog	regular frog
"regular"	10	0
"dart"	0	10

• Risk of deciding "regular" given new observation x is

$$\sum_{j} L[j \rightarrow \operatorname{reg}] P_{Y|X}(j \mid x) =$$

$$= L[\operatorname{reg} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{reg} \mid x) + L[\operatorname{dart} \rightarrow \operatorname{reg}] P_{Y|X}(\operatorname{dart} \mid x)$$

$$= 0 \times 0.9 + 10 \times 0.1 = 1$$

• Info dart-snake has given new x

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$

Dart-Snake Losses

snake prediction	dart frog	regular frog
regular	10	0
dart	0	10

• Risk of deciding "dart" given x is

$$\sum_{j} L[j \rightarrow dart] P_{Y|X}(j \mid x) =$$

$$= L[reg \rightarrow dart] P_{Y|X}(reg \mid x) + L[dart \rightarrow dart] P_{Y|X}(dart \mid x)$$

$$= 10 \times 0.9 + 0 \times 0.1 = 9$$

- The dart-snake optimally decides *"regular"* given x
- Once again, this is consistent with the probabilities

• In summary, if both snakes have

$$P_{Y|X}(j \mid x) = \begin{cases} 0 & j = \text{dart} \\ 1 & j = \text{regular} \end{cases}$$

then both say "regular"

• However, if

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$

- the vulnerable snake decides "dart"
- the predator snake decides "regular"





• The infinite loss for saying regular when frog is dart, makes the vulnerable snake much more cautious!

(Conditional) Risk, Loss, & Probability

• Note that the only factors involved in the *Risk*

$$R(x,i) = \sum_{j} L[j \to i] P_{Y|X}(j \mid x)$$

are

- the Loss Function

$$L[i \rightarrow j]$$

- and the *Measurement-Conditional Probabilities*

$$P_{Y|X}(j \mid x)$$

- The risk is the *expected loss* of the decision ("on *average*, you will loose this much!")
- The risk is not necessarily zero!

(Conditional) Risk, Loss, & Probability

• The *best* that the "vulnerable" ordinary snake can do when

$$P_{Y|X}(j \mid x) = \begin{cases} 0.1 & j = \text{dart} \\ 0.9 & j = \text{regular} \end{cases}$$

is to always decide "dart" and accept the loss of 9

- Clearly, because starvation will lead to death, a more realistic loss function for an ordinary snake would have to:
 - Account for how hungry the snake is. (If the snake is starving, it will have to be more risk preferring.)
 - Assign a finite cost to the choice of "regular" when the frog is a dart.
 (Maybe dart frogs will only make the snake super sick sometimes.)
- In general, the loss function is not "learned"
 - You know how much mistakes will cost you, or assess that in some way
 - What if I can't do that? -- one reasonable default is the 0/1 loss function

0/1 Loss Function

- This is the case where we assign
 - i) zero loss for no error and ii) equal loss for the two error types

$$L[i \rightarrow j] = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases}$$

snake prediction	dart frog	regular frog
"regular"	1	0
"dart"	0	1

• Under the 0/1 loss:

$$i^{*}(x) = \arg\min_{i} \sum_{j} L[j \rightarrow i] P_{Y|X}(j \mid x)$$
$$= \arg\min_{i} \sum_{j \neq i} P_{Y|X}(j \mid x)$$

0/1 Loss Function

• Equivalently:

$$i^{*}(x) = \arg\min_{i} \sum_{j \neq i} P_{Y|X}(j \mid x)$$
$$= \arg\min_{i} \left[1 - P_{Y|X}(i \mid x)\right]$$
$$= \arg\max_{i} P_{Y|X}(i \mid x)$$

- Thus the Optimal Decision Rule is
 - Pick the class that has largest posterior probability given the observation x. (I.e., pick the most probable class)
- This is the Bayes Decision Rule (BDR) for the 0/1 loss
 - We will simplify our discussion by assuming this loss, but you should always be aware that other losses may be used

0/1 Loss Function

• The risk of this optimal decision is

$$R(x, i^{*}(x)) = \sum_{j} L[j \to i^{*}(x)] P_{Y|X}(j \mid x)$$
$$= \sum_{j \neq i^{*}(x)} P_{Y|X}(j \mid x)$$
$$= 1 - P_{Y|X}(i^{*}(x) \mid x)$$

- This is the probability that Y is *different* from *i**(*x*) given *x*, which is *the x-conditional probability that the optimal decision is wrong*.
- The expected Optimal Risk $R = E_X[R(x,i^*(x))]$ is the probability of error of the optimal decision

