Probability Theory

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Probability Theory in Machine Learning

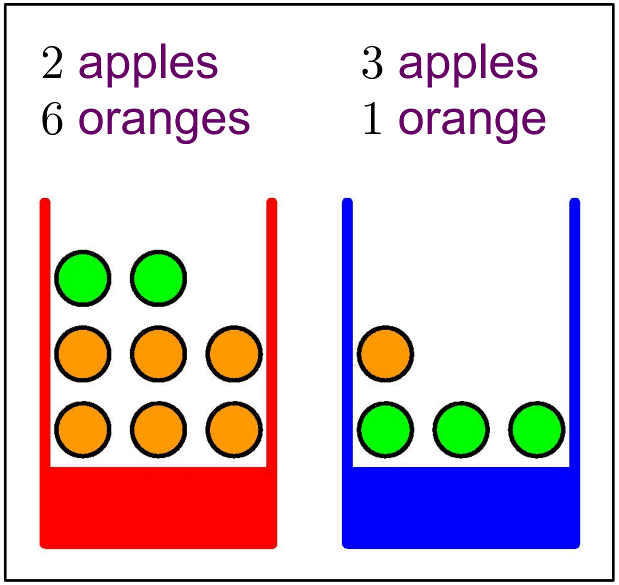
- Probability is key concept is dealing with uncertainty
  - Arises due to finite size of data sets and noise on measurements
- Probability Theory
  - Framework for quantification and manipulation of uncertainty
  - One of the central foundations of machine learning

Random Variable (R.V.)

- Takes values subject to chance
  - E.g., X is the result of coin toss with values $Head$ and $Tail$ which are non - numeric
    - X can be denoted by a r.v. x which has values of 1 and 0
  - Each value of x has an associated probability
- Probability Distribution
  - Mathematical function that describes
    1. possible values of a r.v.
    2. and associated probabilities

Probability with Two Variables

- Key concepts:
  - conditional & joint probabilities of variables
- Random Variables: B and F
  - Box B, Fruit F
    - F has two values orange (o) or apple (a)
    - B has values red (r) or blue (b)



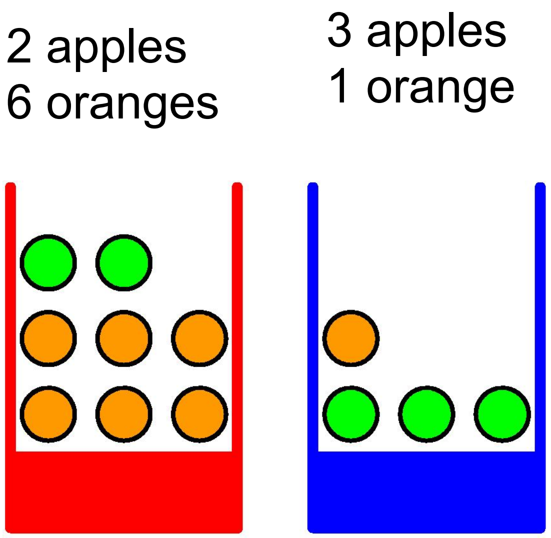
$P(F{=}o){=}3/4$ and $P(F{=}a){=}1/4$

Let $p(B{=}r){=}4/10$ and $p(B{=}b){=}6/10$

Given the above data we are interested in several probabilities of interest: *marginal, conditional and joint* Described next

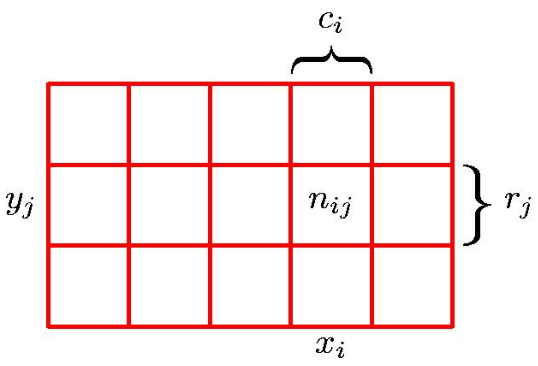
Probabilities of Interest

- Marginal Probability
  - what is the probability of an apple? $P(F=a)$
    - Note that we have to consider $P(B)$
- Conditional Probability
  - Given that we have an orange what is the probability that we chose the blue box? $P(B=b|F=o)$
- Joint Probability
  - What is the probability of orange AND blue box? $P(B=b,F=o)$



Sum Rule of Probability Theory

- Consider two random variables
- X can take on values x_i, i=1,, M
- Y can take on values y_i, i=1,..L
- N trials sampling both X and Y
- No of trials with X=x_i and Y=y_j is n_{ij}



Joint Probability $p(X=x_i, Y=y_j)=\frac{n_{ij}}{N}$

- Marginal Probability $p(X=x_i)=\frac{c_i}{N}$

Since $c_i=\sum_j n_{ij}$, $\boxed{p(X=x_i)=\sum_{j=1}^{L} p(X=x_i, Y=y_j)}$

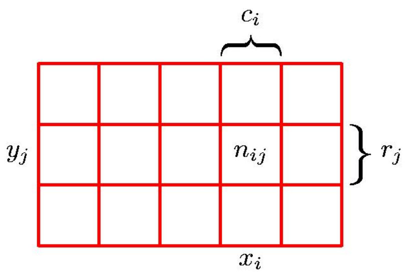
Product Rule of Probability Theory

- Consider only those instances for which $X=x_i$
- Then fraction of those instances for which $Y=y_j$ is written as $p(Y=y_j|X=x_i)$
- Called conditional probability
- Relationship between joint and conditional probability:

$$p(Y = y_j \mid X = x_i) = \frac{n_{ij}}{c_i}$$

$$\boxed{p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}} = \frac{n_{ij}}{ci} \bullet \frac{c_i}{N}$$

$$= \boxed{p(Y = y_j \mid X = x_i) p(X = x_i)}$$



Bayes Theorem

- From the product rule together with the symmetry property $p(X,Y)=p(Y,X)$ we get

$$p(Y \mid X) = \frac{p(X \mid Y)p(Y)}{p(X)}$$

- Which is called Bayes' theorem
- Using the sum rule the denominator is expressed as

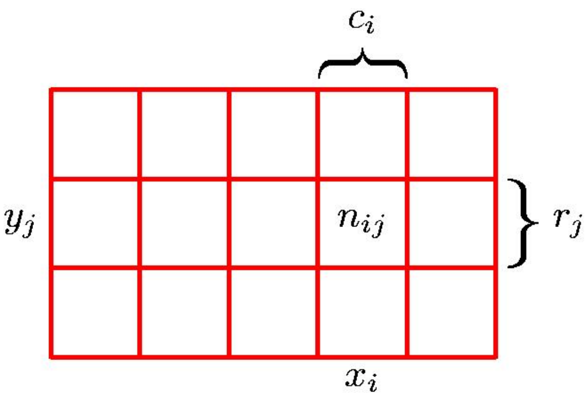
$$p(X) = \sum_{Y} p(X \mid Y)p(Y)$$

Normalization constant to ensure sum of conditional probability on LHS sums to 1 over all values of Y

Rules of Probability

- Given random variables X and Y
- Sum Rule gives Marginal Probability

$$p(X = x_i) = \sum_{j=1}^{L} p(X = x_i, Y = y_j) = \frac{c_i}{N}$$



- Product Rule: joint probability in terms of conditional and marginal

$$p(X,Y) = \frac{n_{ij}}{N} = p(Y \mid X)p(X) = \frac{n_{ij}}{c_i} \times \frac{c_i}{N}$$

- Combining we get Bayes Rule

$$p(Y \mid X) = \frac{p(X \mid Y)p(Y)}{p(X)}$$

where

$$p(X) = \sum_{Y} p(X \mid Y)p(Y)$$

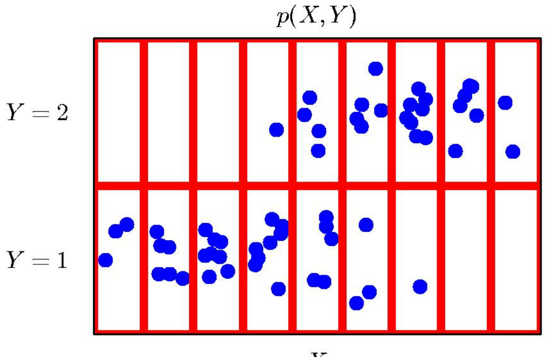
Viewed as

Posterior a likelihood x prior

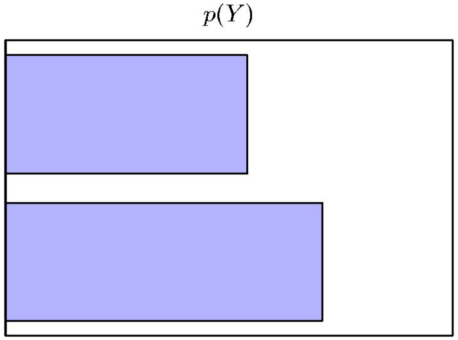
Ex: Joint Distribution over two Variables

X takes nine possible values, Y takes two values

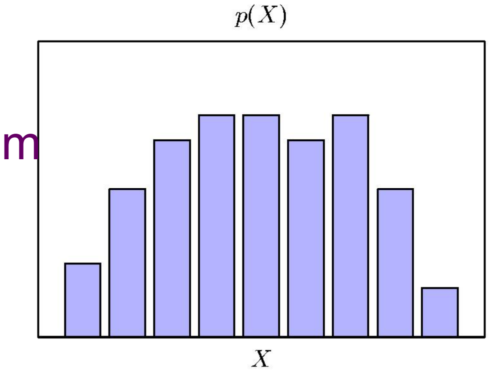
$N = 60$ data points



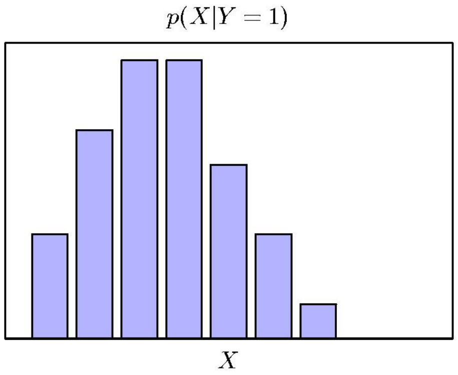
Histogram of Y (Fraction of data points having each value of Y)



Histogram of X



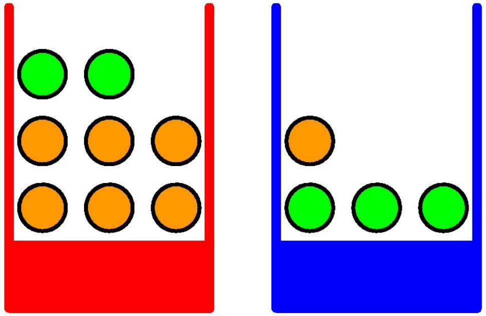
Histogram of X given Y=1



Fractions would equal the probability as N →oo

Bayes rule applied to Fruit Problem

- Probability that box is red given that fruit picked is orange



$$p(B=r \mid F=o) = \frac{p(F=o \mid B=r)\,p(B=r)}{p(F=o)}$$

$$= \frac{\frac{3}{4} \times \frac{4}{10}}{\frac{9}{20}} = \boxed{\frac{2}{3} = 0.66}$$

The *a posteriori* probability of 0.66 is different from the *a priori* probability of 0.4

- Probability that fruit is orange
  - From sum and product rules

$$p(F=o) = p(F=o,B=r) + p(F=o,B=b)$$

$$= p(F=o \mid B=r)\,p(B=r) + p(F=o \mid B=b)\,p(B=b)$$

$$= \frac{6}{8} \times \frac{4}{10} + \frac{1}{4} \times \frac{6}{10} = \boxed{\frac{9}{20} = 0.45}$$

The *marginal* probability of 0.45 is lower than average probability of 7/12=0.58

Independent Variables

- If $p(X,Y)=p(X)p(Y)$ then X and Y are said to be independent
- Why?
- From product rule: $\boxed{p(Y \mid X) = \frac{p(X,Y)}{p(X)} = p(Y)}$

- In fruit example if each box contained same fraction of apples and oranges then $p(F|B)=p(F)$

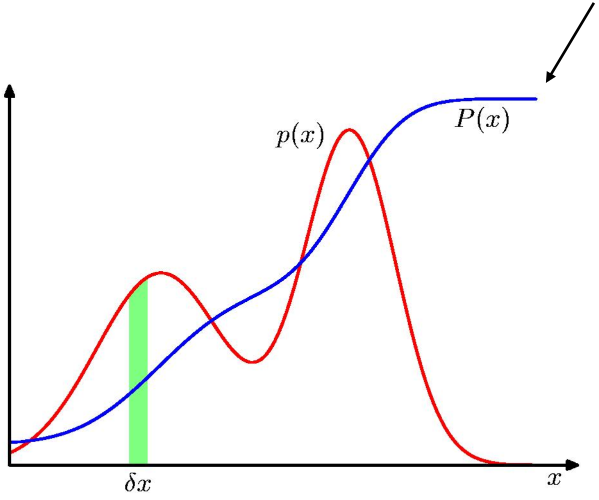
Probability Density Function (pdf)

- Continuous Variables
- If probability that x falls in interval $(x, x+\delta x)$ is given by $p(x)\,dx$ for δx → 0

  then $p(x)$ is a pdf of x
- Probability x lies in interval (a,b) is

$$p(x \in (a,b)) = \int_a^b p(x)\,dx$$

Cumulative Distribution Function



Probability that x lies in Interval $(-\infty, z)$ is

$$P(z) = \int_{-\infty}^{z} p(x)\,dx$$

Several Variables

- If there are several continuous variables $x_1,\ldots,x_D$ denoted by vector x then we can define a joint probability density $p(\mathrm{x})=p(x_1,..,x_D)$
- Multivariate probability density must satisfy

$$p(\mathrm{x}) \geq 0$$

$$\int_{-\infty}^{\infty} p(\mathrm{x})\, d\mathrm{x} = 1$$

Sum, Product, Bayes for Continuous

- Rules apply for continuous, or combinations of discrete and continuous variables

$$p(x) = \int p(x, y)\, dy$$

$$p(x, y) = p(y \mid x) p(x)$$

$$p(y \mid x) = \frac{p(x \mid y) p(y)}{p(x)}$$

- Formal justification of sum, product rules for continuous variables requires measure theory

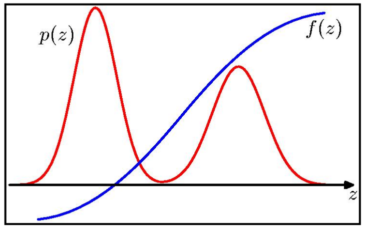
Expectation

- Expectation is *average* value of some function $f(x)$ under the probability distribution $p(x)$ denoted $E[f]$
- For a discrete distribution

$$E[f] = \Sigma_x p(x)\ f(x)$$

- For a continuous distribution

$$E[f] = \int p(x) f(x)\, dx$$



Examples of $f(x)$ of use in ML:

$f(x)=x$; $E[f]$ is mean

$f(x)=\ln\ p(x)$; $E[f]$ is entropy

$f(x)=-\ln[q(x)/p(x)]$; K-L divergence

- If there are N points drawn from a pdf, then expectation can be approximated as

$$E[f] = (1/N)\Sigma_n{}^N{}_{=1}\ f(x_n)$$

This approximation is extremely important when we use sampling to determine expected value

- Conditional Expectation with respect to a conditional distribution

$$E_x[f] = \Sigma_x p(x|y)\ f(x)$$

Variance

- Measures how much variability there is in $f(x)$ around its mean value $E[f(x)]$
- Variance of $f(x)$ is denoted as

$$\mathrm{var}[f] = E[(f(x) - E[f(x)])^2]$$

- *Expanding the square*

$$\mathrm{var}[f] = E[(f(x)^2] - E[f(x)]^2$$

- Variance of the variable x itself

$$\mathrm{var}[x] = E[x^2] - E[x]^2$$

Covariance

- For two random variables x and y their covariance is
- $$\mathrm{cov}[x,y] = E_{x,y}\left[\{x\text{-}E[x]\}\ \{y\text{-}E[y]\}\right]$$
  $$= E_{x,y}[xy]\ \text{-}\ E[x]E[y]$$
  - Expresses how x and y vary together
- If x and y are independent then their covariance vanishes
- If x and y are two vectors of random variables covariance is a matrix
- If we consider covariance of components of vector x with each other then we denote it as $\mathrm{cov}[x] = \mathrm{cov}\,[x,x]$

Bayesian Probabilities

- Classical or Frequentist view of Probabilities
  - Probability is frequency of random, repeatable event
  - Frequency of a tossed coin coming up heads is $1/2$
- Bayesian View
  - Probability is a quantification of uncertainty
  - Degree of belief in propositions that do not involve random variables
  - Examples of uncertain events as probabilities:
    - Whether Arctic Sea ice cap will disappear
    - Whether moon was once in its own orbit around the sun
    - Whether Thomas Jefferson had a child by one of his slaves
    - Whether a signature on a check is genuine

Bayesian Representation of Uncertainty

- Use of probability to represent uncertainty is not an ad-hoc choice
- If numerical values are used to represent degrees of belief, then simple set of axioms for manipulating degrees of belief leads to sum and product rules of probability (Cox’ s theorem)
- Probability theory can be regarded as an extension of Boolean logic to situations involving uncertainty (Jaynes)

Bayesian Approach

- Quantify uncertainty around choice of parameters $\mathbf{w}$
  - E.g., w is vector of parameters in curve fitting

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

- Uncertainty before observing data expressed by $p(\mathbf{w})$
- Given observed data $D = \{\ t_1, \ .\ .\ t_N\}$
  - Uncertainty in w after observing D, by Bayes rule:

$$\boxed{p(\mathbf{w}\mid D) = \frac{p(D\mid \mathbf{w})p(\mathbf{w})}{p(D)}}$$

  - Quantity $p(D|\mathbf{w})$ is evaluated for observed data
    - It can be viewed as function of $\mathbf{w}$
    - It represents how probable the data set is for different parameters $\mathbf{w}$
    - It is called the *Likelihood function*
    - Not a probability distribution over $\mathbf{w}$

Bayes theorem in words

- Uncertainty in $\mathbf{w}$ expressed as

$$p(\mathbf{w} \mid D) = \frac{p(D \mid \mathbf{w})p(\mathbf{w})}{p(D)}$$

- Bayes theorem in words:

$$\text{posterior} \;\; \alpha \;\; \text{likelihood} \times \text{prior}$$

- Denominator is normalization factor
  - Involves marginalization over w

$$p(D) = \int p(D \mid \mathbf{w})p(\mathbf{w})\, d\mathbf{w} \quad \text{by Sum Rule}$$

Role of Likelihood Function

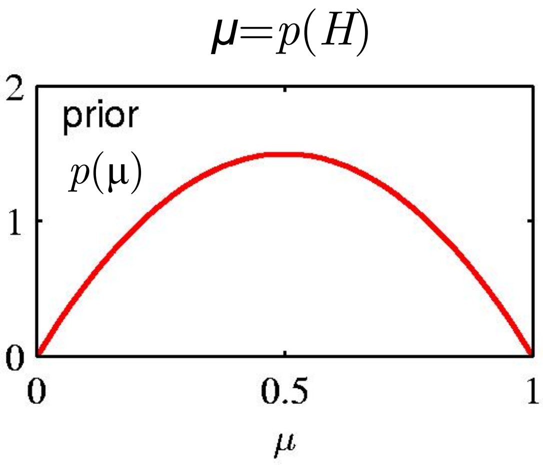
- Likelihood Function plays central role in both *Bayesian* and *frequentist* paradigms
- Frequentist:
  - $\mathbf{w}$ is a fixed parameter determined by an estimator;
  - Error bars on estimate are obtained from possible data sets D
- Bayesian:
  - There is a single data set D
  - Uncertainty in parameters expressed as probability distribution over $\mathbf{w}$

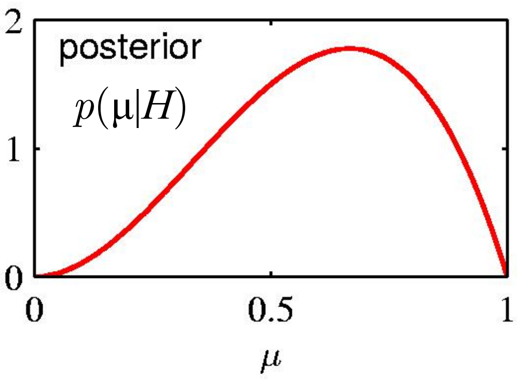
Maximum Likelihood Approach

- In frequentist setting w is a fixed parameter
  - w is set to value that maximizes likelihood function $p(D|\mathrm{w})$
  - In ML, negative log of likelihood function is called error function since maximizing likelihood is equivalent to minimizing error
- Error Bars
  - Bootstrap approach to creating L data sets
    - From N data points new data sets are created by drawing N points at random with replacement
    - Repeat L times to generate L data sets
    - Accuracy of parameter estimate can be evaluated by variability of predictions between different bootstrap sets

Bayesian: Prior and Posterior

- Inclusion of prior knowledge arises naturally
- Coin Toss Example
  - Fair looking coin is tossed three times and lands Head each time
  - Classical m.l.e of the probability of landing heads is 1 implying all future tosses will land $Heads$
  - Bayesian approach with reasonable prior will lead to less extreme conclusion





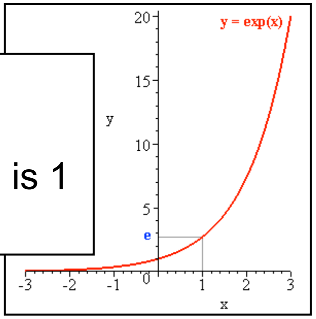
Practicality of Bayesian Approach

- Marginalization over whole parameter space is required to make predictions or compare models
- Factors making it practical:
    - Sampling Methods such as *Markov Chain Monte Carlo* methods
    - Increased speed and memory of computers
- Deterministic approximation schemes such as *Variational Bayes* and *Expectation propagation* are alternatives to sampling

The Gaussian Distribution

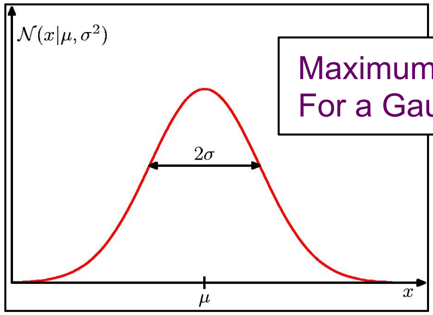
- For single real-valued variable x

$$N(x\mid\mu,\sigma^2)=\frac{1}{(2\pi\sigma^2)^{1/2}}\exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



What is an Exponential:
$y=e^x$, where $e=2.718$
Its value for argument 0 is 1
It is its own derivative

- It has two parameters:
  - Mean μ, variance σ^2,
  - *Standard deviation* σ
    - *Precision* $\beta=1/\sigma^2$



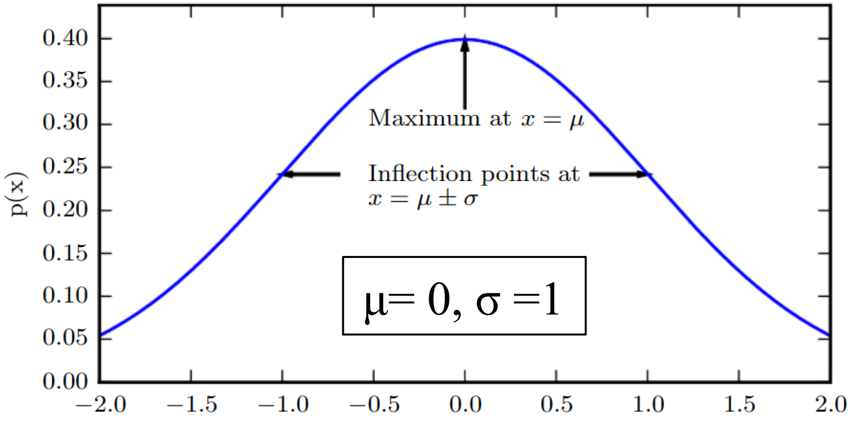
Maximum of a distribution is its mode
For a Gaussian, mode coincides with mean

- Can find expectations of functions of x under Gaussian

$$E[x]=\int_{-\infty}^{\infty}N(x\mid\mu,\sigma^2)$$

$$E[x^2]=\int_{-\infty}^{\infty}N(x\mid\mu,\sigma^2)x^2dx=\mu^2+\sigma^2$$

$$\mathrm{var}[x]=E[x^2]-E[x]^2=\sigma^2$$



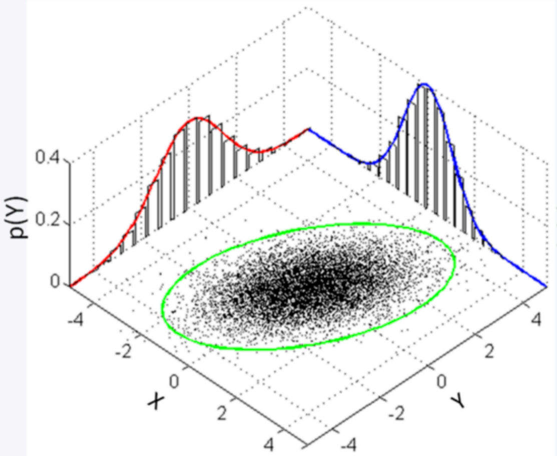
μ= 0, σ =1

Multivariate Gaussian Distribution

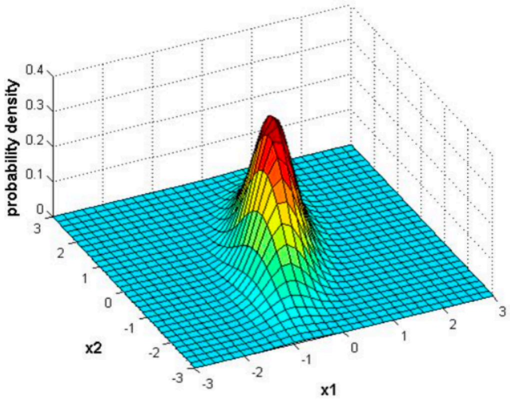
- For single real-valued variable x

$$N(\mathrm{x} \mid \boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{ -\frac{1}{2} (\mathrm{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathrm{x} - \boldsymbol{\mu}) \right\}$$

- It has parameters:
  - Mean $\boldsymbol{\mu}$, a D-dimensional vector
  - Covariance matrix Σ
    - Which is a $D \times D$ matrix



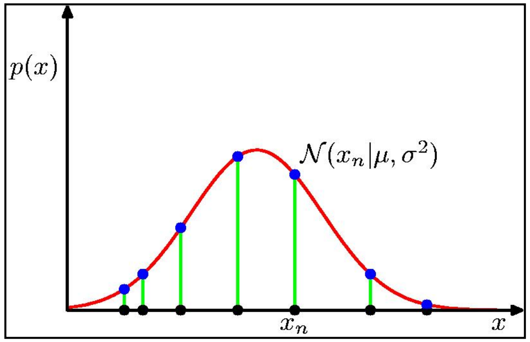
Many sample points from a multivariate normal distribution with $\boldsymbol{\mu} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and $\boldsymbol{\Sigma} = \begin{bmatrix} 1 & 3/5 \\ 3/5 & 2 \end{bmatrix}$, shown along with the 3-sigma ellipse, the two marginal distributions, and the two 1-d histograms.



$$\boldsymbol{\mu} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{bmatrix} 0.25 & 0.3 \\ 0.3 & 1 \end{bmatrix}$$

Likelihood Function for Gaussian



- Given N scalar observations $\mathrm{x}=[x_1,..\ x_n]^{\mathrm{T}}$
  - Which are independent and identically distributed
- Probability of data set is given by likelihood function

$$p(\mathrm{x}\,|\,\mu,\sigma^2)=\prod_{n=1}^{N}N(x_n\,|\,\mu,\sigma^2)$$

Data: black points
Likelihood= product of blue values
Pick mean and variance to maximize this product

- Log-likelihood function is

$$\ln p(\mathrm{x}\,|\,\mu,\sigma^2)=-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu)^2-\frac{N}{2}\ln\sigma^2-\frac{N}{2}\ln(2\pi)$$

- Maximum likelihood solutions are given by

$$\mu_{ML}=\frac{1}{N}\sum_{n=1}^{N}x_n$$ which is the sample mean

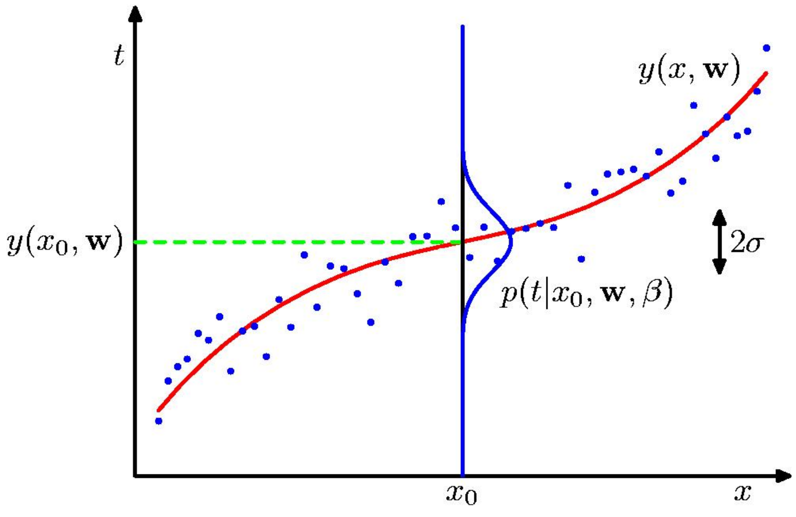
$$\sigma^2_{ML}=\frac{1}{N}\sum_{n=1}^{N}(x_n-\mu_{ML})^2$$ which is the sample variance

Curve Fitting Probabilistically

- Goal is to predict for target variable t given a new value of the input variable x
  - Given N input values $\mathbf{x}=(x_1,..x_N)^{\mathrm{T}}$ and corresponding target values $\mathbf{t}=(t_1,..,t_N)^{\mathrm{T}}$
  - Assume given value of x, value of t has a Gaussian distribution with mean equal to $y(x,\mathbf{w})$ of polynomial curve

$$p(t|x,\mathbf{w},\beta)=N(t|y(x,\mathbf{w}),\beta^{-1})$$

$$\boxed{y(x,\mathbf{w}) = w_0 + w_1x + w_2x^2 + .. + w_Mx^M = \sum_{j=0}^{M} w_jx^j}$$



Gaussian conditional distribution for t given x.
Mean is given by polynomial function $y(x,\mathbf{w})$
Precision given by β

Curve Fitting with Maximum Likelihood

- Likelihood Function is $$p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} N(t_n \mid y(x_n, \mathbf{w}), \beta^{-1})$$
- Logarithm of the Likelihood function is

$$\ln p(\mathbf{t} \mid \mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

- To find maximum likelihood solution for polynomial coefficients $\mathbf{w}_{\mathrm{ML}}$
  - Maximize w.r.t **w**
  - Can omit last two terms -- don't depend on **w**
  - Can replace $\beta/2$ with ½ (since it is constant wrt **w**)
  - Minimize negative log-likelihood
  - Identical to sum-of-squares error function

Precision parameter with MLE

- Maximum likelihood can also be used to determine β of Gaussian conditional distribution
- Maximizing likelihood wrt β gives

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N}\sum_{n=1}^{N}\left\{y(x_n, \mathbf{w}_{\mathrm{ML}}) - t_n\right\}^2$$

- First determine parameter vector $\mathbf{w}_{\mathrm{ML}}$ governing the mean and subsequently use this to find precision β_{ML}

Predictive Distribution

- Knowing parameters $\mathbf{w}$ and β
- Predictions for new values of x can be made using

$$p(t|x,\mathbf{w}_{\mathrm{ML}},\beta_{\mathrm{ML}})=N(t|y(x,\mathbf{w}_{\mathrm{ML}}),\beta_{\mathrm{ML}}{}^{-1})$$

- Instead of a point estimate we are now giving a probability distribution over t

A More Bayesian Treatment

- Introducing a prior distribution over polynomial coefficients $\mathbf{w}$

$$p(\mathbf{w} \mid \alpha) = N(\mathbf{w} \mid 0, \alpha^{-1} I) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right\}$$

  - where α is the precision of the distribution
  - $M+1$ is total no. of parameters for an M^{th} order polynomial
  - α are Model parameters also called *hyperparameter*
    - they control distribution of model parameters

Posterior Distribution

- Using Bayes theorem, posterior distribution for $\mathbf{w}$ is proportional to product of prior distribution and likelihood function

$$p(\mathbf{w}|\mathbf{x},\mathbf{t},\alpha,\beta) \quad \alpha \quad p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)\,p(\mathbf{w}|\alpha)$$

- $\mathbf{w}$ can be determined by finding the most probable value of $\mathbf{w}$ given the data, ie. maximizing posterior distribution
- This is equivalent (by taking logs) to minimizing

$$\frac{\beta}{2}\sum_{n=1}^{N}\left\{y(x_n,\mathbf{w})-t_n\right\}^2+\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}$$

- Same as sum of squared errors function with a regularization parameter given by $\lambda=\alpha/\beta$

Bayesian Curve Fitting

- Previous treatment still makes point estimate of $\mathbf{w}$
  - In fully Bayesian approach consistently apply sum and product rules and integrate over all values of $\mathbf{w}$
- Given training data $\mathbf{x}$ and $\mathbf{t}$ and new test point x , goal is to predict value of t
  - *i.e,* wish to evaluate *predictive distribution* $p(t|x,\mathbf{x},\mathbf{t})$
- Applying sum and product rules of probability
  - Predictive distribution can be written in the form

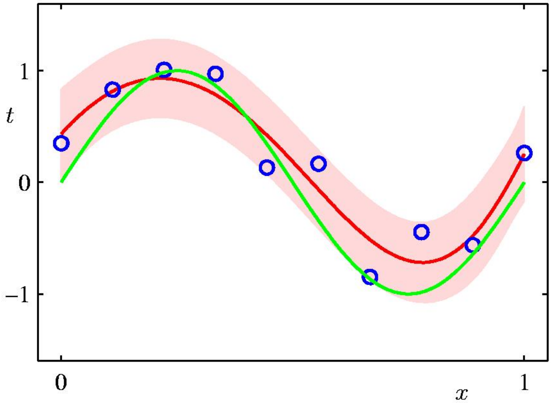
$$\begin{aligned}
p(t\mid x,\mathbf{x},\mathbf{t}) &= \int p(t,\mathbf{w}\,|x,\mathbf{x},\mathbf{t})d\mathrm{w} && \text{by Sum Rule (marginalizing over w)}\\
&= \int p(t|x,\mathbf{w},\mathbf{x},\mathbf{t})\;\, p(\mathrm{w}\mid x,\mathrm{x},\mathbf{t}) && \text{by Product Rule}\\
&= \int \underbrace{p(t|x,\mathbf{w})}_{p(t\mid x,\mathbf{w})=N(t\mid y(x\;,\mathbf{w}),\beta^{-1})}\underbrace{p(\mathbf{w}|\mathbf{x},\mathbf{t})}_{\text{Posterior distribution over parameters Also a Gaussian}}\mathrm{dw} && \text{by eliminating unnecessary variables}
\end{aligned}$$

Bayesian Curve Fitting

- Predictive distribution is also Gaussian

$$p(t \mid x, \mathbf{x}, \mathbf{t}) = N(t \mid m(x), s^2(x))$$

  – Where the Mean and Variance are dependent on x



Predictive Distribution is a M=9 polynomial
α = 5 x 10^{-3}
β =11.1
Red curve is mean
Red region is ± 1 std dev

Model Selection

Models in Curve Fitting

- In polynomial curve fitting:
  - an optimal order of polynomial gives best generalization
- Order of the polynomial controls
  - the number of free parameters in the model and thereby model complexity
- With regularized least squares l also controls model complexity

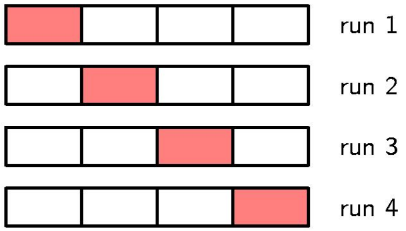
Validation Set to Select Model

- Performance on training set is not a good indicator of predictive performance
- If there is plenty of data,
  - use some of the data to train a range of models Or a given model with a range of values for its parameters
  - Compare them on an independent set, called validation set
  - Select one having best predictive performance
- If data set is small then some over-fitting can occur and it is necessary to keep aside a test set

S-fold Cross Validation

- Supply of data is limited
- All available data is partitioned into S groups
- S-1 groups are used to train and evaluated on remaining group
- Repeat for all S choices of held-out group
- Performance scores from S runs are averaged

S=4



If S=N this is the leave-one-out method

Bayesian Information Criterion

- Criterion for choosing model
- *Akaike Information criterion* (AIC) chooses model for which the quantity

$$\ln p(\mathrm{D}|\mathrm{w}_{\mathrm{ML}}) - \mathrm{M}$$

- Is highest
- Where M is number of adjustable parameters
- BIC is a variant of this quantity

The Curse of Dimensionality

Need to deal with spaces with many variables in machine learning