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Markov Properties of Graph Models and Probabilistic Inference on Bayesian Networks in Genetics

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Abstract

Probability propagation in trees of clusters (PPTC) is an algorithm that provides an easy method for probability inference. It uses the markov properties of graph models, and the underlying graph model is converted into a secondary structure, on which probabilities are calculated. In the present study, the authors illustrate PPTC method by computing probabilities using transition probability matrix (tpm) and using the PPTC algorithm on a simple genetic inheritance model and the results are compared.

AMS Subject Classification:
Keywords: Graph theory, digraphs, recursive factorization of probability on graph models, markov properties, PPTC method.

Introduction

In human genetic research, sophisticated statistical methods are increasingly being used to analyze results, the most widely used one being *Bayesian Inference Method* [11]. Many complex genetic computations can only be performed approximately and involve repeated random sampling techniques, typically in the form of *Markov Chain Monte Carlo (MCMC) methods*. A new technique that is becoming increasingly used in genetic studies is the application of an area in mathematics called *Graph Theory* to map networks of biological interactions. Graphs are an easy way of visualizing these interactions. *Bayesian Networks (BN)* are effective combinations of graph theory and Bayesian probability theory in the study of genetic models. BNs rely on inference algorithms to compute probabilities in the context of observed evidence. One of which is the PPTC algorithm method used in expert systems [10]. PPTC algorithms are of crucial importance to many of the steps within any efficient MCMC algorithm. In the present study, we illustrate the steps involved in a PPTC algorithm on a simple genetic model and compare the probabilities computed by this method with that obtained through the usual markov chain method.

Basic Terminology in Graph Theory

A *graph* $G = (V(G), E(G))$ consists of two finite sets; $V(G)$, the vertex set of the graph, which is a non-empty set of elements called vertices and, $E(G)$, the edge set of the graph, which is a possibly empty set of elements called edges such that each edge e in E is assigned an unordered pair of vertices (u, v), called the end vertices of e [2, 8, 16]. A directed graph or *digraph* $D = (V(D), A(D))$ consists of a non-empty finite set V of vertices and a finite set A of ordered pairs of distinct vertices called arcs. A *walk* is a sequence of edges for getting from one vertex to another, $u \rightarrow v \rightarrow w$. A walk in which no vertex appears more than once is called a *path*. A walk of the form $u \rightarrow v \rightarrow w \rightarrow u$ is called a *cycle*. A graph with no cycles is called an *acyclic graph*. A graph is *connected* if there is a path connecting every two vertices of the graph. Otherwise, it is called a disconnected graph. The set of vertices whose deletion makes the connected graph disconnected is called *separating set*. If the separating set contains only one vertex, v, then, v is called a cut-vertex. A bridge is an edge whose removal makes the connected graph disconnected. If for any vertices v and w of the digraph D, there is a path from v to w, then D is called *strongly connected*. The graph $H = (W, F)$ is a *subgraph* of the graph $G = (V, E)$ if $W \subset V$ and $F \subset E$. A subgraph H of a graph G is a *spanning subgraph* of G if H contains every vertex of G. A graph in which every two vertices is adjacent is called a *complete graph* . A subgraph which is complete is called a *complete subgraph*. A complete subgraph which is not a proper subgraph of any complete subgraph is called a *clique*. *Ancestral set* of a vertex in a digraph is the vertex itself and the set of its ancestors. A vertex u is an ancestor of a vertex v if either u is a parent of v or, u is an ancestor of at least one of the parents of v. The ancestral set of a set of vertices Y is the union of the ancestral sets of the vertices in Y.

Markov Chain and Markov Properties

A process $\{X_n, n = 0, 1, \dots\}$ is called a *markov chain* [7] if, for $j, k, j_1, j_2, \dots, j_{n-1} \in N$, (states of the chain) $P\{X_n = k \mid X_{n-1} = j, X_{n-2} = j_1, \dots, X_0 = j_{n-1}\} = P\{X_n = k \mid X_{n-1} = j\} = p_{jk}$ (called the transition probabilities) and the transition probability matrix (*tpm*) of the chain is given by $P = \begin{pmatrix} p_{11} & p_{12} & \cdots \\ p_{21} & p_{22} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}$.

For r.vs X, Y, Z on a probability space $(\Omega, \mathbb{B}, P)$, $X \coprod Y|Z[P]$, denote, under P, X and Y are *conditionally independent* [3], given Z. When Z is trivial, this becomes

simple independence of X and Y, denoted as $X \coprod Y[P]$.
$X \coprod Y|Z \Rightarrow$

- $P(X \in A, Y \in B \mid Z) = P(X \in A \mid Z)P(Y \in B \mid Z)$ almost surely.
- $P(X \in A|Y, Z) = P(X \in A|Z)$ almost surely.
- $P(X \in A|Y, Z) = a(Z)$ almost surely depending on A.

properties

1. $X \coprod Y|Z \Rightarrow Y \coprod X|Z$
2. $X \coprod Y|X$
3. $X \coprod Y|Z$ and $W = f(Y) \Rightarrow X \coprod W|Z$
4. $X \coprod Y|Z$ and $W = f(Y) \Rightarrow X \coprod Y|(W, Z)$
5. $X \coprod Y|Z$ and $X \coprod W|(Y, Z) \Rightarrow X \coprod (Y, W)|Z$
6. $X \coprod Y|Z$ and $X \coprod Z|Y$
    - $\not\Rightarrow X \coprod (Y, Z)$
    - $\Rightarrow X \coprod (Y, Z)|Y \bigwedge Z$ where $Y \bigwedge Z$ is the common information in Y and Z.

Graph Models of Markov Properties

A model of the markov properties above, is termed a graphoid [11,12,14,15,17]. Let G be an undirected graph with vertex set V. Let $A, B, \ldots$ be subsets of V. $A \coprod_G B \mid C$ if any path joining a vertex in A to one in B must intersect C. Let $X = (X_v : v \in V)$ be a collection of random variables satisfying the graphoid axioms. Let $X_A = (X_v : v \in A)$

(i) X is pairwise markov over G if, whenever there is no edge joining i and j in G so that $i \coprod j \mid V\{i, j\}$, then $X_i \coprod X_j \mid X_{v\{i,j\}}$.

(ii) X is local markov over G if, with δ_i, the set of nearest neighbors of i in G, so that $i \coprod_G V\ \{i\} \mid \delta_i$, then, $X_i \coprod X_{v\ \{i\}} \mid X_{\delta_i}$.

(iii) X is global markov over G if $X_A \coprod X_B \mid X_C$ whenever $A \coprod_G B \mid C$.

Let D be a directed graph with vertex set V. $A \coprod_D B \mid C$ if $A \coprod_{G'} B \mid C$ where G' is the moral graph of D', the smallest ancestral subgraph of D containing $A \cup B \cup C$. If $(X_v : v \in V)$ belong to an arbitrary semi-graphoid,

(i) X is directed markov over D if $X_A \coprod X_B \mid X_C$ whenever $A \coprod_D B \mid C$

(ii) X is local markov over D if for each $v \in V$, $X_v \coprod X_{nd(v)} \mid X_{pa(v)}$ and a weaker version of this is $X_v \coprod X_{pre(v)} \mid X_{pa(v)}$, where $pre(v)$ denotes the set of predecessors of v in some well-numbering of D, while $pa(v)$ denotes the set of parents of v in D, also $v \coprod_D pre(v) \mid pa(v)$; $nd(v)$ is the set of non descendants of v.

Conditional independence and so the markov properties are intimately related to factorization.

Definition 1.1. [12] A probability measure P on $\mathcal{B}$ is said to factorize according to G if for all complete subsets $a \subseteq V$ there exist non-negative functions Ψ_a that depend on x through x_a only, and there exists a product measure $\mu = \bigotimes_{\alpha \in V} \mu_\alpha$ on $\mathcal{B}$ such that, P has density f with respect to μ where f has the form

$$f(x) = \prod_{acomplete} \Psi_a(x).$$

Definition 1.2. [12] A probability distribution P admits a recursive factorization according to a digraph D, if there exist σ-finite measures μ_α over $\mathcal{B}$ and non-negative functions $K^\alpha(.,\ .), \alpha \in V$, henceforth referred to as kernels, defined on $\mathcal{F}_\alpha X \mathcal{B}_{pa(\alpha)}$ such that

$$\int K^\alpha(y_\alpha, x_{pa(\alpha)}) \mu_\alpha(dy_\alpha) = 1$$

and P has density f with respect to the product measure $\mu = \bigotimes_{\alpha \in V} \mu_\alpha$ given by

$$f(x) = \prod_{\alpha \in V} K^\alpha(x_\alpha, x_{pa(\alpha)}$$

. If P admits a recursive factorization as above the kernels $K^\alpha(., x_{pa(\alpha)})$are the densities for the conditional distribution of X_α, given $X_{pa(\alpha)} = x_{pa(\alpha)}$ and thus,

$$f(x) = \prod_{\alpha \in V} f(x_\alpha \mid x_{pa(\alpha)})$$

Lemma 1.3. [12] If P admits a recursive factorization according to the directed acyclic graph D, it factorizes according to moral graph D^m and therefore obeys the global markov property relative to D^m.

Proposition 1.4. [12] If P admits a recursive factorization according to the directed acyclic graph D and A is an ancestral set, then the marginal distribution P_A admits a recursive factorization according to D_A.

Corollary 1.5. [12] Let P factorize recursively according to D. Then, $A \coprod B \mid S$ whenever A and B are separated by S in $(D_{An(A\cup B\cup S)})^m$, the moral graph of the smallest ancestral set containing $A \cup B \cup S$. The property is known as directed global markov property.

Proposition 1.6. [12] Let A, B and S be disjoint subsets of a directed, acyclic graph D. Then S d-separates A from B if and only if S, separates A from B in $(D_{A_n(A\cup B\cup S)})^m$.

The global directed markov property can thus be formulated by requiring that $A \coprod B \mid S$ whenever S d-separates A from B.

BNs and Inference on BNs

A Bayesian network for $X = \{X_1, X_2, \ldots, X_n\}$ consists of a directed acyclic graph(DAG) where the vertex set is X and, a set of conditional probabilities, $P = \{p(X_i \mid pa(X_i))\}$ - Conditional probability distributions of variables X_i given its parents in the graph. In a BN, conditional independence properties can be used to simplify the general factorization formula for the joint probability and the result is a factorization that can be expressed by the use of DAGs. Thus a BN is a DAG, whose structure defines a set of conditional independence properties. These properties can be found using graphical manipulations, such as d-separation. To each vertex is associated a conditional probability distribution, conditioning being on the parents of the vertex. The joint density over the set of all variables is then given by $P(X) = \prod_i p(X_i \mid pa(X_i))$. This is called a *recursive factorization according to the DAG.* This factorization is equivalent to the general factorization but takes into account the conditional independence properties of the DAG in simplifying individual terms in the product of the general factorization. Only if the DAG is complete, will this formula and the general factorization coincide. The BNs rely on inference algorithms to compute posterior probabilities in the context of observed evidence. One established method for probability inference on BNs is the Probability Propagation in Trees of Clusters (PPTC) algorithm, as developed by Lauritzen and Spiegelhalter and refined by Jensen *et al.* [10]. The aim of the algorithm is to use the model specified by the joint distribution to calculate marginal distributions conditional on some observation of one or more variables. The process of constructing the inference engine from the model specification is sometimes called *compiling the model.* The manipulations required are almost all graphical. There are five stages in the graphical manipulations namely,

1. Marrying Parents: Add undirected edges to all co-parents which are not currently joined

2. Constructing the Moral Graph: Drop all directions in the graph obtained from Stage 1. The resultant graph is the moral graph.

3. Triangulating the moral graph: Add sufficient additional undirected links between nodes such that there are no cycles of length 4 or distinct nodes without a short-cut.

4. Identify the cliques(clusters) of this triangulated graph.

5. Formation of Junction Tree: Join the cliques together to form the junction tree (tree of clusters).

The joint density of the vertex set X in a DAG,say D is given by $P(X) = \prod_i p(X_i \mid pa(X_i)) = a(X_i, pa(X_i))$, the conditional probability factors for X_i can be considered as a function of X_i and its parents, called *potential.*

Now after steps 1 and 2 we have an undirected graph, in which for each node both it and the set of its parents in the original graph form a complete subgraph in the moral graph. Hence the original factorization of $P(X)$ on the DAG, D goes over to an equivalent factorization on these complete subsets in the moral graph, D^m. Denote the set of cliques of D^m, by C^m. Then each of the complete subgraphs formed from $\{X_i\} \bigcup pa\{X_i\}$ is contained within at least one clique. Hence, we can form functions a_C such that $P(X) = \prod_{C \in C^m} a_C((X_i)_C)$, where $a_C((X_i)_C)$ is a function of the variables in the clique C. The remaining three steps are required to ensure consistency and efficiency. In step 3, edges are added to D^m, to form a triangulated graph D^t. Adding edges to the graph does not stop a clique of the moral graph formed from being a complete subgraph in D^t. Thus for each clique in C^m, there is at least one clique in the triangulated graph which contains it. Hence we can write $P(X) = \prod_{C \in C^t} a_C(X_i)_C$. Now in step 4, the cliques of D^t are joined to form a junction tree. The important property of the junction tree is the *running intersection property* which means that if variable X_i is contained in two cliques, then it is contained in every clique along the path connecting those two cliques. The edge joining two cliques is called a *separator*. The choice of the tree is immaterial except for computational efficiency considerations. Including functions on the separators, the joint density representation can be $P(X) = \dfrac{\prod_{C \in C^t} a_C(X_i)_C}{\prod_{S \in S^t} b_S(X_i)_S}$, and marginal representation on a clique can be $p(X) = \dfrac{\prod_C p(C)}{\prod_S p(S)}$. Marginals for individual variables can be obtained from these clique marginals by further marginalization.

Markov Chain in Genetics

In the present study, we consider the case of an autosomal dominant gene disorder; A denotes a dominant allele of the gene and a a normal allele. consider a simple pedigree, consisting of a father, a mother and a child. Let X_n denote the genetic state of a child in the n^{th} generation. Then, X_n assumes states AA, Aa, aa with probabilities $q^2, 2pq, p^2$, if, $P(a) = p, P(A) = q; p + q = 1$. Then X_{n-1} can be thought of as the genetic state of one of the parents, say mother and let X'_{n-1} be the genetic state of father. By Hardy-Weinberg law, both X_{n-1} and X'_{n-1} assume states AA, Aa, aa with probabilities $q^2, 2pq, p^2$. X_{n-1} and X'_{n-1} are independent.

$$P(X_n \mid X_{n-1}, X_{n-2}, \ldots, X_0) = P(X_n \mid X_{n-1}), \quad \text{and so,} \quad \{X_n, n \geq 1\} \text{ is a M.C.}$$

$$P(X_n, X'_{n-1} \mid X_{n-1}) = P(X_n \mid X_{n-1}, X'_{n-1})P(X'_{n-1})$$

and hence,

$$P(X_n \mid X_{n-1}) = \sum_{X'_{n-1}} P(X_n, X'_{n-1} \mid X_{n-1}) = \sum_{X'_{n-1}} P(X_n \mid X_{n-1}, X'_{n-1})P(X'_{n-1}).$$

Hence the tpm of the M.C. is given by

$$P = \left(\begin{array}{cccc} & AA & aa & Aa \\ AA & q & 0 & p \\ aa & 0 & p & q \\ Aa & q/2 & p/2 & 1/2 \end{array} \right).$$

Suppose we observed that one person in a population of 2000 persons examined has such a disease. Since it is a dominant gene disorder, persons with both the genotypes Aa and AA will be affected. Hence, $2pq + q^2 = 0.0005$; which gives, $p = 0.99975, q = 0.00025$, and so, the tpm can be written as

$$P = \left(\begin{array}{cccc} & AA & Aa & aa \\ AA & 0.00025 & 0.99975 & 0 \\ Aa & 0.000125 & 0.50000 & 0.499875 \\ aa & 0 & 0.00025 & 0.99975 \end{array} \right).$$

Results

From the above, we can conclude that, if there is no information on the health status of the parents, a child has a 0.05% chance of inheriting the disease ; if one of the parents is known to be affected with the disease, the child has a 50.01% chance of inheriting the same; and if both the parents are known to be affected, the child has a 75% chance of inheriting the disease.

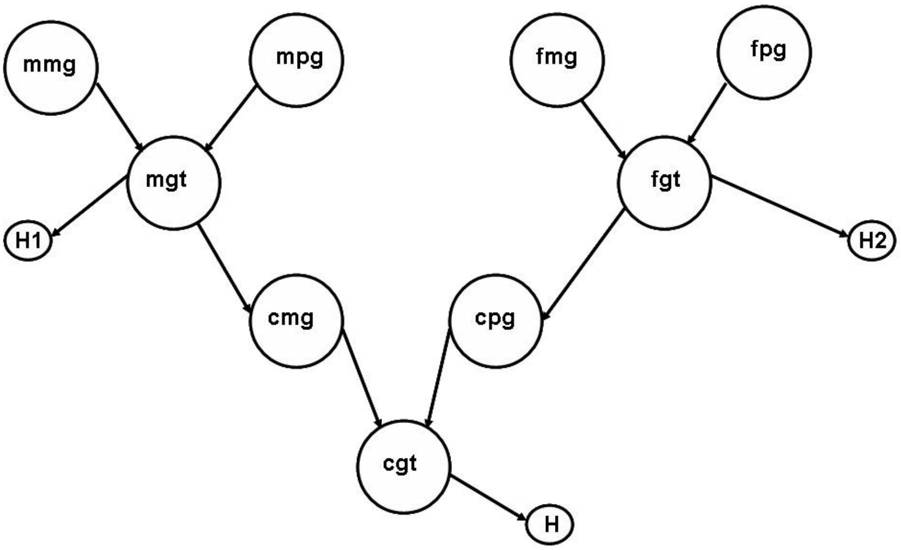

Figure 1: Simple Inheritance Model.

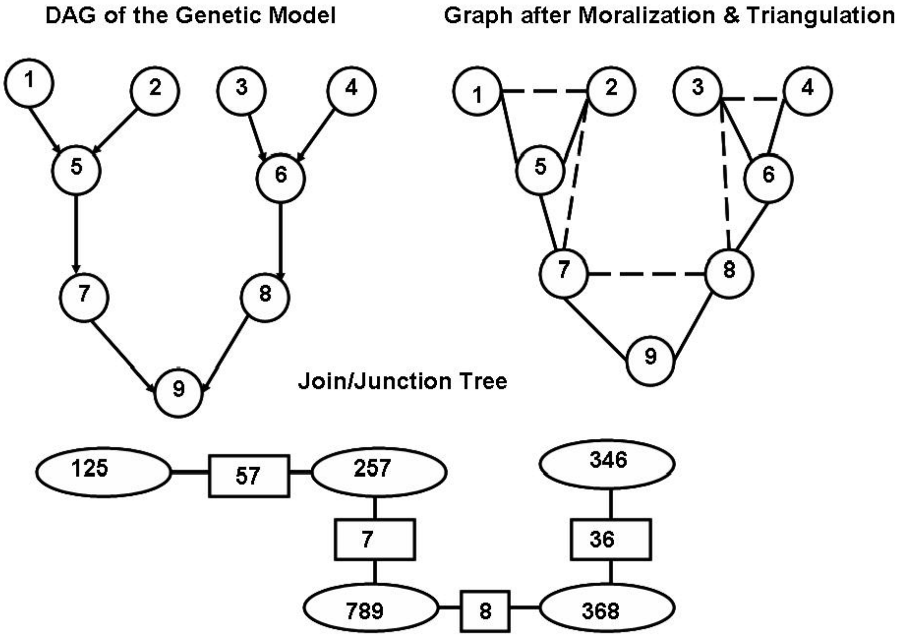

Figure 2: PPTC steps on the Genetic Model.

Table 1: $P(cgt = AA \mid mgt, fgt)$.

mgt/fgt	AA	Aa	aa
AA	1	1/2	0
Aa	1/2	1/4	0
aa	0	0	0

Table 2: $P(cgt = Aa \mid mgt, fgt)$.

mgt/fgt	AA	Aa	aa
AA	0	1/2	1
Aa	1/2	1/2	1/2
aa	1	1/2	0

PPTC Method Applied on the Simple Inheritance Model

The inheritance model, the associated DAG, the triangulated graph and the cluster tree of the pedigree discussed in the previous section are given in Figure 1, and Figure 2; where cgt, cmg, cpg denote child's genotype, child's maternal gene, and child's paternal gene respectively; mgt and fgt are respectively mother's genotype and father's genotype; mmg, mpg, fmg and fpg are mother's maternal gene, mother's paternal gene, father's maternal gene and father's paternal gene respectively. H, $H1$, and $H2$ are respectively the health status of the child, his mother and his father. $cgt = fgt = mgt = \{AA, Aa, aa\}$, $cmg = cpg = mmg = mpg = fmg = fpg = \{A, a\}$, H, $H1$ and $H2$ take values 1 or 0 as the concerned person is healthy or sick.

$P(cgt = AA \mid mgt, fgt)$ is given in Table 1.$P(cgt = Aa \mid mgt, fgt)$ is given in Table 2.

$P(cgt = aa \mid mgt, fgt)$ is given in Table 3. $P(H = 1 \mid mgt, fgt)$ is given in Table 3.

Table 4 gives the $P(H = 0 \mid mgt, fgt)$. The vertex set is changed to $\{1, 2, 3, 4, 5, 6, 7, 8, 9\}$ excluding H, H_1, H_2 for convenience.

By the recursive factorization on the DAG, $P(1, 2, 3, 4, 5, 6, 7, 8, 9) = P(1)P(2)$

Table 3: $P(cgt = aa \mid mgt, fgt)$.

mgt/fgt	AA	Aa	aa
AA	0	0	0
Aa	0	1/4	1/2
aa	0	1/2	1

Table 4: $P(cgt = AA \, or \, Aa \mid mgt, \, fgt)$.

mgt/fgt	AA	Aa	aa
AA	1	1	1
Aa	1	3/4	1/2
aa	1	1/2	0

Table 5: $P(5 \mid 1, 2) = P(mgt \mid (mmg, mpg))$.

mgt	:	AA	Aa	aa
mpg	mmg	-	-	-
A	a	0	1	0
A	A	1	0	0
a	A	0	1	0
a	a	0	0	1

Table 6: $P(6 \mid 3, 4) = P(fgt \mid (fmg, \, fpg))$.

fgt	:	AA	Aa	aa
fpg	fmg	-	-	-
A	a	0	1	0
A	A	1	0	0
a	A	0	1	0
a	a	0	0	1

Table 7: $P(7 \mid 5) = P(cmg \mid mgt)$.

cmg	A	a
mgt	-	-
AA	1	0
Aa	1/2	1/2
aa	0	1

Table 8: $P(8 \mid 6) = P(cpg \mid fgt)$.

cpg	A	a
fgt	-	-
AA	1	0
Aa	1/2	1/2
aa	0	1

$P(3)P(4)P(5 \mid 1, 2)P(6 \mid 3, 4)P(7 \mid 5)P(8 \mid 6)P(9 \mid 7, 8)$.

Table 9: $P(9 \mid 7, 8) = P(cgt \mid (cmg, cpg)$.

cgt cmg	: cpg	AA -	Aa -	aa -
A	a	0	1	0
A	A	1	0	0
a	A	0	1	0
a	a	0	0	1

Table 10: $P(125) = P(1)P(2)P(5 \mid 1, 2) = P(mmg, mpg, mgt) = P(346) = P(fmg, fpg, fgt)$.

1	2	5	P(1,2,5)
A	A	AA	0
A	a	Aa	0.00025
a	A	aA	0.00025
a	a	aa	0.9995

Available information: 1 in 2000 examined has the disease. Hence, $P(A) = 0.00025$, $P(a) = 0.99975$.

$$P(1) = P(2) = P(3) = P(4) = \begin{pmatrix} states: & A & a \\ prob.: & 0.00025 & 0.99975 \end{pmatrix}$$

Case (1): There is no information on the health status of the parents. The probability computations are given in Table 10 to Table 15.

Result. When no information is available on the health status of the parents, the offspring has 0.05% chance of inheriting the dominant gene and 99.95% chance of not inheriting the same.

Table 11: $P(5) = \sum_{(1,2)} P(125) = P(6) = \sum_{(3,4)} P(346))$.

AA	Aa	aa
0	0.0005	0.9995

Table 12: $P(5, 7) = P(5)P(7 \mid 5) = P(6, 8) = P(6)P(8 \mid 6)$.

5	7	P(57)
AA	A	0
Aa	A	0.00025
aa	A	0
AA	a	0
Aa	a	0.00025
aa	a	0.9995

Table 13: $P(7) = \sum_{5} P(5, 7) = P(8) = \sum_{(} 6)P(6, 8)$.

A	a
0.00025	0.99975

Table 14: $P(7, 8, 9) = P(7)P(8)P(9 \mid 7, 8)$.

7	8	9	P(789)
A	A	AA	0
A	a	Aa	0.00025
a	A	Aa	0.00025
a	a	aa	0.9995

Table 15: $P(9) = \sum_{(7,8)} P(7, 8, 9)$.

AA	Aa	aa
0	0.0005	0.9995

Table 16: $P(5, 7) = P(5)P(7 \mid 5)$.

5	7	P(5,7)
Aa	A	1/2
Aa	a	1/2

Table 17: $P(7 \mid 5)$.

cmg:	A	a
mgt=Aa	1/2	1/2

Table 18: $P(7) = \sum_{5} P(5,7)$.

7	A	a
P(7)	1/2	1/2

Table 19: $P(8)$.

A	a
0.00025	0.99975

Table 20: $P(7,8,9) = P(7)P(8)P(9 \mid 7,8)$.

7	8	9	P(7,8,9)
A	A	AA	0.000125
A	a	Aa	0.499875
a	A	Aa	0.000125
a	a	aa	0.499875

Table 21: $P(9) = \sum_{(7,8)} P(7,8,9)$.

AA	Aa	aa
0.000125	0.5	0.4999

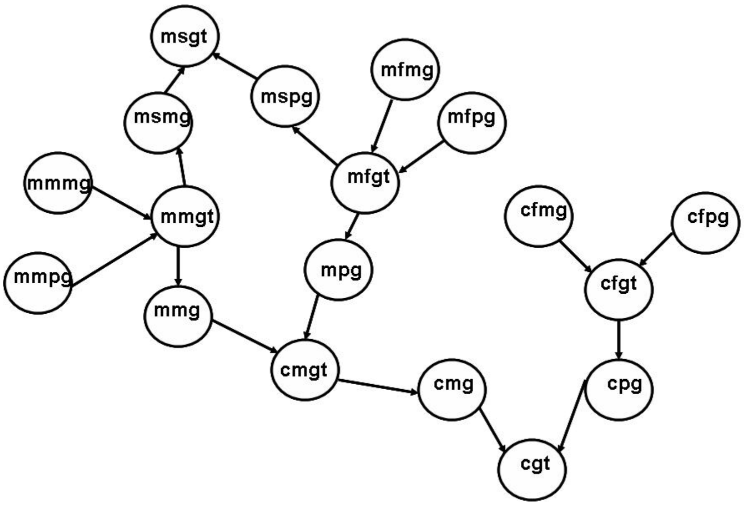

Figure 3: Genetic model including mother's parents and sister.

Case (2): One of the parents, say, mother is known to be sick.

Since $P(AA) = 0, mgt = \{Aa\}$,

5=mgt	Aa	6=fgt	AA	Aa	aa
P(5):	1	P(6):	0	0.0005	0.9995

From Table 21, $P(AA\,or\,Aa) = 0.5001$ and $P(aa) = 0.4999$.

Result: When one of the parents is sick, the offspring has a 50.01% chance of inheriting the disease and 49.99% chance of not inheriting the disease.

case (3): When both the parents are sick, the child has a 75% chance of inheriting the gene, as is seen from Table 4.

Now we consider an extension of the simple inheritance model where mother's parents and sister are also included. The model is given in Figure 3.

Suppose it is observed that mother's sister is sick. This implies that she inherited it from either of her parents or from both.

case(1): When one of the grand parents is sick.

From previous computations,

mgt:	AA	Aa	aa	fgt:	AA	Aa	aa
prob.:	0	0.5001	0.4999	prob.:	0	0.0005	0.9995

Using Table 1, Table 2, Table 3, and Table 4, we could compute
$P(cgt = AA) = 0.000062$, $P(cgt = Aa) = 0.25015$
and so, $P(cgt = AAor\,Aa) = 0.2502$. $P(cgt = aa) = 0.7498$.

case(2): When both the grand parents are affected.

mgt:	AA	Aa	aa	fgt:	AA	Aa	aa
prob.:	0	0.75	0.25	prob.:	0	0.0005	0.9995

Hence, $P(cgt = AA\,or\,Aa) = 0.3752$ and $P(cgt = aa) = 0.6248$.

Result: When it is observed that child's mother's sister is affected with the particular disease, the child has a chance of 25.02% or 37.52% of inheriting the disease, depending on whether one of the grand parents or both the grand parents are affected.

Conclusion

Method based on the PPTC algorithm yields the same results as that given by the usual *tpm* method. These probability computations on more complicated genealogical structures become unwieldy with the usual methods in practise, where softwares such as SUPERLINK, HUGIN [6, 11, 12]which use PPTC algorithm come handy.

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