Gaussian processes and tree graphs

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1 Introduction

This talk presents the cluster expansion story. In the following $\mathcal{X}$ is a discrete space. In a given situation we shall usually be considering only a finite subset $\Lambda \subseteq \mathcal{X}$. The idea is to get expansions for quantities related to

$$Z_\lambda = \langle e^{S_\Lambda(\phi)} \rangle = e^{F_\Lambda}. \tag{1}$$

The bracket denotes Gaussian expectation. Here the interaction $S(\phi)$ has the local form

$$S_\Lambda(\phi) = \sum_{x \in \Lambda} S_x(\phi) = \sum_{x \in \Lambda} \sum_{n=0}^{m} s_{xn} \phi_x^n. \tag{2}$$

The leading coefficients satisfy $s_{xm} < 0$. This makes $S(\phi)$ bounded above, and so $e^{S(\phi)}$ is bounded. The coefficients s_{x0} are going to be used in the following to cancel the contributions of one point sets. Let

$$f_x(\phi_x) = \exp(S_x(\phi_x)). \tag{3}$$

Then the interaction factor is

$$f_\Lambda(\phi) = \prod_x f_x(\phi_x) = \exp(\sum_x S_x(\phi_x)) = \exp(S_\Lambda(\phi)). \tag{4}$$

The partition function is

$$Z_\Lambda = \langle f_\Lambda(\phi) \rangle = \langle \prod_{x \in \Lambda} f_x(\phi_x) \rangle. \tag{5}$$

This is a moment of the family of random variables $f_x(\phi_x)$.

There are two stages in the analysis. The first is to use the combinatorial exponential. The idea is to expand the moment as a sum of cumulants

$$Z_\Lambda = \sum_{\Gamma \in \mathrm{Part}[\Lambda]} \prod_{A \in \Gamma} K_A. \tag{6}$$

Here Γ is a partition of Λ.

The second stage is to write $Z_\lambda = e^{F_\Lambda}$ as an exponential. This is done as follows. Normalize the $f_x(\phi_x)$ so that each $\langle f_x(\phi_x)\rangle = 1$. Then the one-point subsets may be removed, and so we may write the partition function as

$$Z_\Lambda = \sum_\Delta \mathrm{disjoint}(\Delta) \prod_{A\in\Delta} K_A. \tag{7}$$

Here Δ ranges over collections of subsets A of Λ, each subset having at least two points. Here the A belong to the set $\mathcal{P}(\Lambda)$ of finite subsets of Λ each having at least two elements. This is a power series (actually a polynomial) in the variables K_A of the first stage. Not only that, this series, regarded as a function of these variables, is defined in a way that is entirely combinatorial. It makes no mention of anything about the sets other than the condition that they are disjoint. In this situation it has been shown that it is possible to find a reasonably nice representation

$$F_\Lambda = \sum_{N\neq 0} \frac{1}{N!} c(N) K^N. \tag{8}$$

Because of the combinatorial origin of this expression, the coefficients $c(N)$ are integers.

Standard cluster expansion results have the following consequence. Suppose that we have the rooted tree bound

$$Q = \sup_x \sum_{x\in A} K_A e^{|A|} \leq 1. \tag{9}$$

Then the series for F_Λ converges absolutely, in particular

$$|F_\Lambda| \leq Q|\Lambda|. \tag{10}$$

The main work for the first stage is to establish this rooted tree bound.

There is some similarity between the two stages. In the first stage there is a formal expression for Z_Λ as a sum indexed by graphs inside Λ, and for K_A as a sum indexed by connected graphs inside A. The estimates on the K_A are made possible by replacing the sum over connected graphs by a sum over tree graphs. These estimates depend on assumptions on the covariances C_{xy} and on the interactions. However, unlike the situation with Feynman diagrams, the graph structure does not depend on the detailed structure of the interactions. In particular, the degree of a vertex can be arbitrarily high.

In the second stage there is a formal expression for Z_Λ as a sum indexed by graphs of arbitrary size, and for F_Λ as a sum indexed by connected graphs of arbitrary size. The estimates are made possible by replacing the sum over connected graphs by a sum over tree graphs. These estimates are universal; all they depend on is the sizes of the various K_A.

2 The combinatorial exponential

The key to the rooted tree bound is the forest formula for Gaussian expectations. There is an excellent treatment in [2]. A more general formulation of forest formulas appears in [4]. We are interested in Gaussian expectations with covariance C_{xy}. The idea is to interpolate the covariances with parameters s_{xy} ranging from 0 to 1. When $x \neq y$ we take $s_{xy} = s_{yx} = s_\ell$, where $\ell = \{x, y\}$. We take $s_{xx} = 1$. The corresponding covariance will be denoted $\langle F(\phi)\rangle^s$. As before, we write

$$\Delta_\ell = C_{xy} \frac{\partial}{\partial \phi_x} \frac{\partial}{\partial \phi_y}. \tag{11}$$

The forest formula deals with Gaussian random variables ϕ_x for $x \in \Lambda$. It states that

$$\langle f_\Lambda(\phi)\rangle = \sum_{F \in \mathrm{Forest}[\Lambda]} \int_{[0,1]^F} \langle \left(\prod_{\ell \in F} \Delta_\ell \right) f_\Lambda(\phi)\rangle^{\sigma_F(u)} \prod_{\ell \in F} du_\ell. \tag{12}$$

The forest graph breaks into tree graph components. The quantity $\sigma_F(u)_\ell = 0$ if ℓ links vertices in different components. This means that the Gaussian random variables corresponding to such vertices are independents. On the other hand, if $\ell = \{x, y\}$ links two vertices in the same component, then $\sigma_F(u)_\ell$ is the minimum of the $u_{\ell'}$, where ℓ' ranges over the edges in the unique minimal path in the forest joining x with y.

The proof of the forest formula consists of a systematic iteration of the fundamental theory of calculus. One begins with the empty forest, then considers forests consisting of one edge, then of two edges, and so on. Once one gets to three edges it is necessary to take care to avoid cycles. It turns out it is possible to build the forests in this way, avoiding cycles, until finally one arrives at tree graphs. These are the forest graphs that connect the vertex set, in other words, the maximal forest graphs.

Thus an arbitrary Gaussian expectation is written as a sum over forest graphs. Each graph contribution is a uniform average over a cube indexed by the edges of the forest graph of certain interpolated Gaussian expectations.

Since every forest breaks into tree components, there is a corresponding tree formula. Take $f_A(\phi) = \prod_{x \in A} f_x(\phi_x)$. The tree formula states that

$$K_A = \sum_{T \in \mathrm{Tree}[A]} \int_{[0,1]^T} \langle \left(\prod_{\ell \in T} \Delta_\ell \right) F_A(\phi)\rangle^{\sigma_T(u)} \prod_{\ell \in T} du_\ell. \tag{13}$$

If $\ell = \{x, y\}$ links two vertices, then $\sigma_F(u)_\ell$ is the minimum of the $u_{\ell'}$, where ℓ' ranges over the edges in the unique minimal path in the tree joining x with y.

The hypotheses are formulated as a rather general condition on the covariance together with a rather restrictive condition on the interaction. Both conditions are relatively natural, and they interact well in the course of the proof.

The covariance condition is that

$$\sum_y |C_{xy}| \leq C. \tag{14}$$

The uniform analyticity condition is that for $k \geq 1$ we have

$$|\frac{\partial^k}{\partial \phi^k} F_x(\phi)| \leq \lambda^k k!. \tag{15}$$

Our task is to use these condition to estimate $Q = \sup_x \sum_{x \in A} K_A e^{|A|}$. The result is that if λ is sufficiently small, then we have the rooted tree bound $Q \leq 1$.

From the tree formula we conclude that

$$|K_A| \leq \sum_{T \in \mathrm{Tree}[A]} \prod_{\ell \in T} |C_\ell| \prod_{x \in A} \lambda^{d_x^T} d_x^T!. \tag{16}$$

Fix x in Λ. We need to estimate

$$\sum_{x \in A,\ |A|=n} |K_A| \leq \sum_{T \in \mathrm{Tree}[A]} \sum_{x \in A,\ |A|=n} \prod_{\ell \in T} |C_\ell| \prod_{x \in A} \lambda^{d_x^T} d_x^T!. \tag{17}$$

We can write

$$\sum_{x \in A,\ |A|=n} |K_A| \leq \sum_{T \in \mathrm{Tree}[U_n]} \frac{1}{(n-1)!} \sum_{a: U_n \to \Lambda,\ a(1)=x} \prod_{\{i,j\} \in T} |C_{a(i)\,a(j)}| \prod_{i=1}^n \lambda^{d_i^T} d_i^T!. \tag{18}$$

This gives

$$\sum_{x \in A,\ |A|=n} |K_A| \leq \frac{1}{(n-1)!} C^{n-1} \sum_{T \in \mathrm{Tree}[U_n]} \prod_{i=1}^n \lambda^{d_i^T} d_i^T!. \tag{19}$$

In more detail,

$$\sum_{x \in A,\ |A|=n} |K_A| \leq \frac{1}{(n-1)!} C^{n-1} \sum_{d_1,\ldots,d_n} \sum_{T \in \mathrm{Tree}[U_n; d_1,\ldots,d_n]} \prod_{i=1}^n \lambda^{d_i} d_i!. \tag{20}$$

This looks bad, because of the factorials. For instance, if we replace the sum over trees with given degrees with the sum over trees, then we have to deal with

$$\sum_{d_1,\ldots,d_n} \prod_{i=1}^n \lambda^{d_i} d_i! \leq \left(\sum_{k=1}^{\infty} \lambda^k k! \right)^n. \tag{21}$$

This is not a convergent series.

The factorials are handled by the following device, which is nicely explained in [1]. A result of Cayley shows that the number of trees with given degree function is given by the multinomial coefficient.

$$\#\mathrm{Tree}[U_n; d_1, \ldots, d_n] = \frac{(n-2)!}{\prod_{i=1}^n (d_i - 1)!}. \tag{22}$$

The result is that

$$\sum_{x\in A,\ |A|=n} |K_A| \leq \frac{1}{n-1} C^{n-1} \sum_{d_1,\ldots,d_n} \prod_{i=1}^{n} \lambda^{d_i} d_i. \tag{23}$$

It follows that

$$\sum_{x\in A,\ |A|=n} |K_A| \leq \frac{1}{n-1} C^{n-1} \left(\sum_{k=1}^{\infty} k\lambda^k \right)^n. \tag{24}$$

The conclusion is that

$$\sum_{x\in A,} |K_A| \leq \sum_{n=2}^{\infty} \frac{1}{n-1} C^{n-1} \left(\sum_{k=1}^{\infty} k\lambda^k \right)^n. \tag{25}$$

If λ is sufficiently small, then this is bounded by 1. This is the desired rooted tree bound.

3 The exponential

The method of cluster expansions has a long history; there is a review in [3]. We have the expansion

$$Z_\Lambda = \sum_{\Delta} \prod_{A\in\Delta} K_A. \tag{26}$$

We can write this in tensor form as

$$Z_\Lambda = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{A_1,\ldots,A_n} \mathrm{disjoint}(A_1,\ldots,A_n) K_{A_1} \cdots K_{A_n}. \tag{27}$$

where

$$\mathrm{disjoint}(A_1,\ldots,A_n) = \prod_{\{i,j\}} 1_{A_i\cap A_j=\emptyset} = \sum_{G} \prod_{\{i,j\}\in G} (-1_{A_i\cap A_j\neq\emptyset}) \tag{28}$$

Here the A_i belong to the set $\mathcal{P}(\Lambda)$ of finite subsets of Λ each having at least two elements. The coefficient is non-zero only when the sets do not overlap. In particular, the $A_1,\ldots,A_n$ map from U_n to $\mathcal{P}(\Lambda)$ is bijective. In the graph sum the graph G has vertex set U_n, and the only terms in the graph sum that contribute are from graphs where every edge has corresponding sets that do overlap. The graph sum involves only ± 1 terms, and there is a huge amount of cancellation. Thus $Z_\Lambda = e^{F_\Lambda}$, where

$$F_\Lambda = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{A_1,\ldots,A_n} c(A_1,\ldots,A_n) K_{A_1} \cdots K_{A_n}, \tag{29}$$

and

$$c(A_1, \ldots, A_n) = \sum_{G_c} \prod_{\{i,j\} \in G_c} (-1_{A_i \cap A_j \neq \emptyset}) \tag{30}$$

Here the connected graph G_c has vertex set U_n, and the only terms in the graph sum that contribute are from graphs where every edge has a corresponding overlap. The graph sum involves only ± 1 terms, and there is a still lot of cancellation, though this is now less obvious.

The sum over connected graphs is huge and difficult to estimate directly. We need a resummation that does a lot of the cancellation. The forest and tree formulas formula work to do this. The first idea is to apply the forest formula to the sum of graphs. This involves the application of the forest formula to the function

$$g^s(A_1, \ldots, A_n) = \prod_{\{i,j\}} (1 - s_{\{i,j\}} 1_{A_i \cap A_j \neq \emptyset}). \tag{31}$$

The result is that

$$g^1(A_1, \ldots, A_n) = \sum_F \int_{[0,1]^F} \prod_{\{i,j\} \in F} (-1_{A_i \cap A_j \neq \emptyset}) \prod_{\{i,j\} \notin F} (1 - \sigma^F(u)_{\{i,j\}} 1_{A_i \cap A_j \neq \emptyset}) \prod_{\{i,j\} \in F} du_{\{i,j\}}. \tag{32}$$

The sum over graphs on the left hand side has been written as a much smaller sum over forests on the right hand side. The main idea is to use the corresponding formula for the sum of connected graphs. The result is that

$$c(A_1, \ldots, A_n) = \sum_T \int_{[0,1]^T} \prod_{\{i,j\} \in T} (-1_{A_i \cap A_j \neq \emptyset}) \prod_{\{i,j\} \notin T} (1 - \sigma^T(u)_{\{i,j\}} 1_{A_i \cap A_j \neq \emptyset}) \prod_{\{i,j\} \in T} du_{\{i,j\}}. \tag{33}$$

The sum over connected graphs on the left hand side has been written as a much smaller sum over trees on the right hand side.

The tree formula leads immediately to the tree bound

$$|c(A_1, \ldots, A_n)| \leq \sum_T \prod_{\{i,j\} \in T} 1_{A_i \cap A_j \neq \emptyset}. \tag{34}$$

The main consequence is a bound on the exponential generating function for trees rooted at some point i of color B. The quantity of interest is

$$T_B^\bullet = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{A_1, \ldots, A_n} \#\{i \mid A_i = B\} [\sum_T \prod_{\{i,j\} \in T} 1_{A_i \cap A_j \neq \emptyset}] \prod_{i \in U_n} |K_{A_i}|. \tag{35}$$

This is the exponential generating function for rooted colored trees, where the color palette consists of sets with two or more elements. The root has color B. The weight of an edge $\{i, j\}$ in the tree is 1 or zero depending on whether the corresponding sets overlap or not. The recursive structure of rooted trees gives the fixed point relation

$$T_B^\bullet = |K_B| \exp(\sum_{A \cap B \neq \emptyset} T_A^\bullet). \tag{36}$$

The rooted tree bound $\sum_{x\in A} |K_A|e^{|A|} \leq Q \leq 1$ may be stated in the equivalent form

$$\sum_{A\cap B\neq\emptyset} |K_A|e^{|A|} \leq Q|B|. \tag{37}$$

with $Q \leq 1$. In particular, we have

$$K_B \exp(\sum_{A\cap B\neq\emptyset} |K_A|e^{|A|}) \leq K_B e^{|B|}. \tag{38}$$

This gives an upper bound on the fixed point

$$T^\bullet_A \leq K_A e^{|A|}. \tag{39}$$

Let us write F_Λ in multi-index form as

$$F_\Lambda = \sum_{N\neq 0} \frac{1}{N!} c(N) K^N. \tag{40}$$

Here each N is a multi-index on the set $\mathcal{P}(\Lambda)$ of subsets of Λ, each with at least two elements. Each such N is supported on subsets of Λ. The machinery of cluster expansions above shows that if this condition is satisfied, then for each fixed set $A \subseteq \Lambda$ in $\mathcal{P}(\Lambda)$ we have an estimate on the series pinned at set A of the form

$$\sum_{N\neq 0} \frac{1}{N!} N(A)|c(N)||K|^N \leq T^\bullet_A \leq |K_A|e^{|A|}. \tag{41}$$

It follows that for every $B \subseteq \Lambda$ in $\mathcal{P}(\Lambda)$ we have an estimate on the series pinned near B of the form

$$\sum_{N\neq 0} \frac{1}{N!} [\sum_{A\cap B\neq\emptyset} N(A)]|c(N)||K|^N \leq Q|B|. \tag{42}$$

Define the overlap set O_B as the set of multi-indices N on Λ for which there exists $A \subseteq \Lambda$ with $A \cap B \neq \emptyset$ and $N(A) \geq 1$. Then N in O_B implies $1 \leq \sum_{A\cap B\neq\emptyset} N(A)$. It follows that with this notion of pinning near B we have

$$\sum_{N\in O_B} \frac{1}{N!} |c(N)||K|^N \leq Q|B|. \tag{43}$$

In particular, if we take $B = \Lambda$, then for $N \neq 0$ we have $N \in O_\Lambda$, so

$$|F_\Lambda| \leq \sum_{N\neq 0} \frac{1}{N!} |c(N)||K|^N \leq Q|\Lambda|. \tag{44}$$

4 Appendix on uniform analyticity

Consider the polynomial

$$S(x) = \sum_{n=0}^{m} s_n x^n \tag{45}$$

with $s_m < 0$. In this section we show that if we scale the coefficients of the polynomial to make them small, then we get the uniform analyticity condition for $f(x) = e^{S(x)}$ with a small parameter.

Let a be a parameter with $0 < a \leq 1$. Write $a^m S(x) = S_a(u)$, where $u = ax$. We have

$$S_a(u) = \sum_{n=0}^{m} s_n a^{m-n} u^n. \tag{46}$$

We shall show there is a constant M such that the kth derivative of $e^{S_a(u)}$ is uniformly bounded by M. Consider $S(z)$ as a function of a complex variable z in the strip $|\Im z| \leq 1$. Then because of the sign of the leading coefficient, there is a c such that for $|\Re z| > c$ we have $\Re S_a(z) < 0$, uniformly in a. On the other hand, by compactness there is a C such that for $|\Im z| \leq 1$ and $|\Re z| \leq c$ and $0 \leq a \leq 1$ we have $\Re S_a(x) \leq C$. It follows that $|e^{S_a(z))}| \leq M = e^C$ in the strip, uniformly in a.

Now we can write

$$\frac{d^k}{du^k} e^{S_a(u)} = \frac{k!}{2\pi i} \int \frac{e^{S_a(z)}}{(z-u)^{k+1}}\, dz \tag{47}$$

where the integral is on the unit circle centered at u. This representation gives the bound $Mk!$. It then follows from $u = ax$ that the kth derivative of $e^{a^m S(x)} = e^{S_a(u)}$ is uniformly bounded by Ma^k.

5 Appendix on trees with given degree assignment

If G is a graph on a vertex set V, then the sum of the degrees of the vertices is twice the number of edges. In particular, if T is a tree on vertex set V with n elements, then it has $n-1$ edges, and the sum of the degrees is $2(n-1)$.

In the following it will be convenient to define the *reduced degree* of a vertex as the one less than the degree of the vertex. If T is a tree on vertex set V, then the sum of the reduced degrees of the vertices is $2(n-1) - n = n - 2$. The only contribution to this sum is from the vertices of the tree that are not leaves. The reduced degree is an measure of how far the vertex is from being a leaf. We may think of this reduced degree as a function $R : V \to \mathbf{N}$.

Theorem (Cayley): Let V be a vertex set with n elements. Then there is a bijection from the set of trees on V to the set of functions from $\{1, \ldots, n-2\}$ to V. As a consequence, there are n^{n-2} trees on V.

The function $p : \{1, \ldots, n-2\} \to V$ determining the tree is called the *Prüfer sequence* of the tree. This sequence determines a corresponding multi-index $R : V \to \mathbf{N}$ that counts the number of times each element of V is assumed by this function. The p sequence actually contains more detailed information about the tree, as is shown in the following result.

Theorem (Cayley): Let V be a vertex set with n elements. Then there is a bijection from the set of trees on V to the set of functions from $\{1, \ldots, n-2\}$ to V. The bijection sends the set of trees with given reduced degree function R on V to the set of functions p from $\{1, \ldots, n-2\}$ to V that whose induced multi-index is R. As a consequence, the number of trees with reduced degree function R is the multinomial coefficient

$$\frac{(n-2)!}{R!} = \frac{(n-2)!}{\prod_v r(v)!}. \tag{48}$$

Proof: The task is to produce a bijection from the set of trees on V to the set of lists $v_1, \ldots, v_{n-2}$ of elements from V. Choose a linear order on the vertex set V. The bijection will be defined relative to this linear order. The basic idea is clear: repeatedly prune the tree by removing a leaf and the corresponding edge.

Consider a tree $T_0 = T$ on $V_0 = V$. If we are given T_{i-1} a tree on V_{i-1}, let α_i be the least vertex in V_{i-1} that is a leaf of T_{i-1}. Let v_i be the non-leaf neighbor of α_i in T_{i-1}. Then removing α_i from V_{i-1} and removing the edge joining α_i to v_i gives a new vertex set V_i and a new tree T_i.

This process terminates at $i = n-2$ with V_i having two points and T_i having a single edge. The list $\alpha_1, \ldots, \alpha_{n-2}$ is an injection from $\{1, \ldots, n-2\}$ to V that omits the two points. The list $v_1, \ldots, v_{n-2}$ enumerates the non-leaf element of T according to their reduced degree.

It may be shown that $v_i, \ldots, v_{n-2}$ enumerates the non-leaf elements of T_i and hence the non-leaf elements of T_{i-1}. Thus we can use the sequence $v_1, \ldots, v_{n-2}$ to reconstruct the tree via a reverse process. Given vertices α_j for $j < i$, define α_i to be the least vertex that is not one of these preceding α_j and that is not one of the $v_j, \ldots, v_{n-2}$. The sequence $\alpha_1, \ldots, \alpha_{n-2}$ is an injection from $\{1, \ldots, n-2\}$ to V. The edges of T include the $n-2$ pairs α_i, v_i. To get the full T add the remaining edge joining the two vertices that are not in the range of α.

Notice that at stage i the edge that has been removed in the forward process is the edge that is has been added in the reverse process. So at each stage the set of remaining edges in the forward process is the complement of the set of edges that have been introduced in the reverse process.

Example: Consider the ordered vertex set $\{a, b, c, d, e, f\}$. Consider the tree with two neighboring vertices of degree three, namely b with neighbors a, d, e and d with neighbors b, c, f. Find the corresponding Prüfer sequence of vertices v_1, v_2, v_3, v_4.

Example: Consider the ordered vertex set $\{a, b, c, d, e, f\}$. Consider the Prüfer sequence v_1, v_2, v_3, v_4 with $v_1 = v_3 = b$, $v_2 = v_4 = d$. Find the corresponding tree.

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