A Gentle Introduction to Cluster Expansions

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3. The equilibrium lattice gas

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   - Cluster estimates
   - Abstract polymer systems

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1. Exponential and combinatorial exponential

$\mathcal{P}$ countable set

For each multi-index $N : \mathcal{P} \to \{0, 1, 2, 3, \ldots\}$ with finite support:

factorial $N! = \prod_p N(p)!$

given coefficient $K(N)$ with $K(0) = 1$.

For each $p \in \mathcal{P}$ a variable $w(p)$.

$w^N = \prod_p w(p)^{N(p)}$

For $\Lambda \subset \mathcal{P}$ a finite set define:

$w_\Lambda(p) = w(p)$ for $p \in \Lambda$, otherwise zero.

Define local power series (exponential generating function):

$$Z_\Lambda(w) = \sum_N \frac{1}{N!} K(N) w_\Lambda^N.$$

$$Z_\Lambda(w) = \exp(F_\Lambda(w)).$$

$$F_\Lambda(w) = \sum_M \frac{1}{M!} C(M) w_\Lambda^M.$$

M is a cluster, $C(M)$ is a cluster coefficient.

Combinatorial exponential (cluster expansion):

$$K(N) = \sum_{k=0}^{\infty} \frac{1}{k!} \sum \frac{N!}{M_1! \cdots M_k!} C(M_1) \cdots C(M_k).$$

Inner sum over sequences $M_1 + \cdots + M_k = N$ with each $M_j \neq 0$.

$K(0) = 1$ and $C(0) = 0$.

$|N| = 1$ gives $K(N) = C(N)$

$|N| = 2$ gives $K(N) = C(N) + C(M_1)C(M_2)$ where $M_1 + M_2 = N$, etc.

$$F_\Lambda(w) = \log(Z_\Lambda(w)).$$

Combinatorial logarithm:

$$C(M) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \sum \frac{M!}{N_1! \cdots N_k!} K(N_1) \cdots K(N_k).$$

Inner sum over sequences $N_1 + \cdots + N_k = M$ with each $N_j \neq 0$.

$C(0) = 0$

$|M| = 1$ gives $C(M) = K(M)$

$|M| = 2$ gives $C(M) = K(M) - K(N_1)K(N_2)$ where $N_1 + N_2 = M$, etc.

Combinatorial exponential for sets:

Consider terms with $0 \leq N \leq 1$. Set $K(X) = K(N)$ with X the support of N.

$$K(X) = \sum_{\Gamma=\{Y_1,\ldots,Y_k\}} C(Y_1)\cdots C(Y_k).$$

$\Gamma = \{Y_1, \ldots, Y_k\}$ is a partition of X into disjoint non-empty sets $Y_1, \ldots, Y_k$ with union X.

$K(\{p\}) = C(\{p\})$.

$K(\{p, q\}) = C(\{p, q\}) + C(\{p\})C(\{q\})$.

$K(\{p, q, r\}) = C(\{p, q, r\}) + [C(\{p, q\})C(\{r\}) + \cdots] + C(\{p\})C(\{q\})C(\{r\})$.

Combinatorial logarithm for sets:

$$C(Y) = \sum_{n=1}^{\infty} (-1)^n (n-1)! \sum_{\Delta} K(X_1) \cdots K(X_n)$$

with $\Delta = \{X_1, \ldots, X_n\}$ a partition of Y.

$C(\{p\}) = K(\{p\})$.

$C(\{p,q\}) = K(\{p,q\}) - K(\{p\})K(\{q\})$.

$C(\{p,q,r\}) = K(\{p,q,r\}) - [K(\{p,q\})K(\{r\}) + \cdots] + 2K(\{p\})K(\{q\})K(\{r\})$.

Combinatorial setting for general case:

Let U be an index set with n elements. A colored set is a function $a : U \to \mathcal{P}$.

Interpretation 1: U is an index set, and $\mathcal{P}$ is a set of colors. Then a is a coloring of U.

Interpretation 2: U is a set of particles, and $\mathcal{P}$ is a set of locations. Then a is a particle configuration.

Each colored set a defines a multi-index N_a on $\mathcal{P}$ by $N_a(p) = \#a^{-1}(p)$.

$K(a) = K(N_a)$.

$$Z_\Lambda(w) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{a:U_n \to \mathcal{P}} K(a) \prod_{j \in U_n} w_\Lambda(a(j))$$

Here the U_n in the nth term is a fixed index set with n elements.

Combinatorial exponential for general case:

$$Z_\Lambda(w) = \exp(F_\Lambda(w)).$$

$$Z_\Lambda(w) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{a:U_n \to \mathcal{P}} K(a) \prod_{j \in U_n} w(a(j)).$$

$$F_\Lambda(w) = \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{b:V_m \to \mathcal{P}} C(b) \prod_{j \in V_m} w(b(j)).$$

Let $a = a_U : U \to \mathcal{P}$. Combinatorial exponential:

$$K(a_U) = \sum_{\Gamma = \{V_1, \ldots, V_k\}} C(a_{V_1}) \cdots C(a_{V_k}).$$

Here a_V is the restriction of a_U to $V \subset U$.

$\Gamma = \{V_1, \ldots, V_k\}$ is a partition of U into disjoint non-empty sets $V_1, \ldots, V_k$ with union U.

Partition the sets; keep the colors!

2. Cumulant expansions

Fundamental problem of mathematical physics: μ expectation associated with measure on space of large dimension. $\rho > 0$ is a positive function. Control new measure μ' with expectation

$$\mu'(f) = \frac{\mu(f\rho)}{\mu(\rho)}.$$

Technique: $\rho = \prod_{p \in \Lambda} \lambda_p$. Control the dependence of the λ_p. Get estimates uniform in Λ.

Method 1: Write $\lambda_p = \exp(-\beta_p U_p)$. Use ordinary exponential with cumulants of the U_p.

Method 2: Use combinatorial exponential with cumulants of the λ_p.

Method 1: $\lambda_p = \exp(-\beta_p U_p)$. Calculate using the cumulants of the U_p.

Write $tf = \sum_{j \in J} t_j f_j$ and $\beta U = \sum_{p \in \Lambda} \beta_p U_p$.

$$\mu'(\exp(tf)) = \frac{\mu(\exp(tf - \beta U))}{\mu(\exp(-\beta U))}.$$

$$Z'_J(t) = \frac{Z_{J,\Lambda}(t, -\beta)}{Z_\Lambda(-\beta)}.$$

$$F'_J(t) = F_{J,\Lambda}(t, -\beta) - F_\Lambda(-\beta).$$

Spectacular cancellation between numerator and denominator!

The μ' cumulants of the f_j are expressed in terms of the μ cumulants of the f_j and U_p by

$$C'(L) = \sum_M \frac{1}{M!} C(L, M)(-\beta)^M.$$

for $L \neq 0$, where the sum is over all M.

Method 2.

$$\mu'(f) = \frac{\mu(f\rho)}{\mu(\rho)}.$$

Use directly $\rho = \prod_{p \in \Lambda} \lambda_p$

Calculate using the cumulants of the λ_j.

$$\mu'(\prod_{j \in J} f_j) = \frac{\mu(\prod_{j \in J} f_j \prod_{p \in \Lambda} \lambda_j)}{\mu(\prod_{p \in \Lambda} \lambda_j)}.$$

$$K'(J) = \frac{K(J, \Lambda)}{K(\Lambda)}.$$

$$K'(J) = \frac{\sum_{\Gamma \subset J \sqcup \Lambda} \prod_{Y \in \Gamma} C(Y)}{\sum_{\Gamma \subset \Lambda} \prod_{Y \in \Gamma} C(Y)}.$$

Problem: Cancellation between numerator and denominator?

3. The equilibrium lattice gas

$\mathcal{P}$ is set of sites, while $N : \mathcal{P} \to \{0, 1, 2, 3, \ldots\}$ is number of particles per site. The variable $w(p)$ is activity: prior weight for a particle at p. The coefficient $K(N)$ is a particle interaction factor.

discrete probablity density:

$$P_\Lambda(N) = \frac{1}{Z_\Lambda(w)} \frac{1}{N!} K(N) w_\Lambda^N.$$

Poisson example: $K(N) = 1$ for all N.

$$Z_\Lambda(w) = \exp(\sum_{p \in \Lambda} w(p)).$$

$N(p)$ is Poisson with mean $w(p)$.

Bernoulli example: $K(N) = 1$ for $1 \leq N \leq 1$.

$$Z_\Lambda(w) = \prod_{p \in \Lambda} (1+w(p)) = \exp(\sum_{p \in \Lambda} \log(1+w(p))).$$

$N(p)$ is Bernoulli with probability of success $w(p)/(1 + w(p))$.

Recall $Z_\Lambda(w) = \exp(F_\Lambda(w))$.

The w are activities.

$Z_\Lambda(w)$ is the partition function.

$F_\Lambda(w)$ is the pressure.

First Mayer equation. Expected number of particles at site p in terms of pressure:

$$\frac{1}{Z_\Lambda(w)} w(p) \frac{\partial}{\partial w(p)} Z_\Lambda(w) = w(p) \frac{\partial}{\partial w(p)} F_\Lambda(w).$$

$$\frac{1}{Z_\Lambda(w)} \sum_N N(p) \frac{1}{N!} K(N) w_\Lambda^N = \sum_M M(p) \frac{1}{M!} C(M) w_\Lambda^M.$$

Two-site interaction: $0 \leq t(p, q) \leq 1$.

$t(p, q) = t(q, p)$

Pairs of particles at two different sites: $L_{\{p,q\}}(N) = N(p)N(q)$ for $p \neq q$.

Pairs of particles at same site: $L_{\{p,q\}}(N) = \binom{N(p)}{2}$ for $p = q$.

total interaction between all pairs of particles:

$$K(N) = \prod_{\{p,q\}} (1 - t(p, q))^{L_{\{p,q\}}(N)}.$$

The weight of a configuration N is decreased by a factor $(1-t(p, q))$ for each pair of particles at sites p, q.

Partition function equation. Derivative of partition function in terms of modified activities:

$$\frac{\partial}{\partial w(p)} Z_\Lambda(w) = Z_\Lambda((1 - t_p)w).$$

Proof: Add one particle at p. This changes the particle configuration to $N^{+p}(r) = N(r) + \delta_{pr}$.

Then the number of pairs of particles at p, q increases to $L_{\{p,q\}}(N^{+p}) = L_{\{p,q\}}(N) + N(q)$.

One more particle at p decreases the weight of the configuration N by a factor of $1 - t(p,q)$ for each single particle at q. The total decrease is $\prod_q (1 - t(p,q))^{N(q)} = (1 - t_p)^N$, where t_p is the function $t_p(q) = t(p,q)$.

The interaction with one more particle is given by $K(N^{+p}) = K(N)(1 - t_p)^N$.

$$\sum_N \frac{1}{N!} K(N^{+p}) w_\Lambda^N = \sum_N \frac{1}{N!} K(N)(1 - t_p)^N w_\Lambda^N.$$

Second Mayer equation. Expected number of particles in terms of modified activities:

$$w(p)\frac{\partial}{\partial w(p)}F_\Lambda(w) = \exp(F_\Lambda((1-t_p)w)-F_\Lambda(w)).$$

$$\sum_M M(p)\frac{C(M)}{M!}w_\Lambda^M = w(p)\exp(-\sum_M T_p(M)\frac{C(M)}{M!}w_\Lambda^M).$$

where $T_p(M) = 1-(1-t_p)^M$.

Proof: Start with partition function equation. Use first Mayer equation and definition of pressure.

Remark: The $T_p(M)$ factor is nonlinear in t_p and in M.

Let $(tM)(p) = \sum_q t(p,q)M(q)$.

Interaction bound lemma:

$$T_p(M) \leq (tM)(p).$$

Energy bound $A(q) \geq 0$. Expected particle number bound $|w(q)| \exp(A(q))$.

Cluster condition (Kotecký-Preiss version):

$$\sum_q t(p,q)|w(q)| \exp(A(q)) \leq A(p).$$

Stability bound for expected particle number:

$$\sum_M M(q) \frac{1}{M!} |C(M)||w|_\Lambda^M \leq |w(q)| \exp(A(q)).$$

Stability bound for interaction:

$$\sum_M (tM)(p) \frac{1}{M!} |C(M)||w|_\Lambda^M \leq A(p).$$

Expected particle number for infinite system:

$$\frac{1}{Z_\Lambda(w)} \sum_N N(p) \frac{1}{N!} K(N) w_\Lambda^N \to \sum_M M(p) \frac{1}{M!} C(M) w^M$$

as $\Lambda \to \mathcal{P}$.

Proof of stability bound (following Ueltschi):

Let

$$f_k(p) = \sum_{|M|=k} M(p)\frac{1}{M!}|C(M)||w|^M_\Lambda.$$

Prove by induction

$$f_k(p) \leq |w(p)| \,\mathrm{exp}(A(p)).$$

¿From second Mayer equation and interaction bound lemma

$$f_{k+1}(p) \leq |w(p)| \,\mathrm{exp}(\sum_q t(p,q) f_k(q)).$$

By induction

$$f_{k+1}(p) \leq |w(p)| \,\mathrm{exp}(\sum_q t(p,q) w(q) \,\mathrm{exp}(A(q))).$$

¿From the cluster estimate

$$f_{k+1}(p) \leq |w(p)| \,\mathrm{exp}(A(p)).$$

Abstract polymer system: $t(p,q) = 1$ or 0. Also $t(p,p) = 1$.

Incompatible sites: $I(p) = \{q \mid t(p,q) = 1\}$.

$T_p(M) = 1 - (1 - t_p)^M$ is 1 or 0 if $M(I(p)) > 0$ or $= 0$.

Interaction bound lemma: $T_p(M) \leq M(I(p))$.

Second Mayer equation: particle probability in terms of incompatibility

$$\sum_M M(p) \frac{c(M)}{M!} w_\Lambda^M = w(p) \exp(- \sum_{M(I(p))>0} \frac{c(M)}{M!} w_\Lambda^M).$$

Cluster estimate:

$$\sum_{q \in I(p)} |w(q)| \exp(A(q)) \leq A(p).$$

Stability bound for interaction:

$$\sum_M M(I(p)) \frac{1}{M!} |c(M)| |w|_\Lambda^M \leq A(p).$$

4. Combinatorial exponential as exponential

Combinatorial exponential as polymer system:

$$K(X) = \sum_{\Gamma=\{Y_1,\ldots,Y_k\}} C(Y_1)\cdots C(Y_k).$$

The sum is over partitions $\Gamma = \{Y_1, \ldots, Y_k\}$. Each Y_j has at least one point. The Y_j are disjoint. The union of the Y_j is X.

Problem: The union constraint is not a two-site interaction.

Solution: Suppose Y has one point implies $C(Y) = 1$. The sum is now over sets $\Gamma = \{Y_1, \ldots, Y_r\}$. Each Y_j has at least two points. The Y_j are disjoint.

This is a polymer system. The weights are the $C(Y)$. The two-body interaction is the disjointness condition.

Combinatorial exponential as exponential:

Translate from combinatorics to polymer system.

$Y \subset X \sim p \in \Lambda$

$C(Y) \sim w(p)$

$K(X) \sim Z_\Lambda(w)$

$Z \cap Y \neq \emptyset \sim t(q,p) = 1$

Exponential representation:

$$Z_\Lambda(w) = \exp(\sum_M \frac{c(M)}{M!} \prod_{p \in \Lambda} w(p)^{M(p)}).$$

$$K(X) = \exp(\sum_M \frac{c(M)}{M!} \prod_{Z \subset X} C(Z)^{M(Z)}).$$

Recall that

$$K(X) = \sum_{\Gamma=\{Y_1,\ldots,Y_r\}} C(Y_1) \ \cdots C(Y_r).$$

The cluster estimate is

$$\sum_{Z\cap Y\neq\emptyset} C(Z)\,\mathrm{exp}(A(Z)) \leq A(Y).$$

Conclusion: The cluster estimate gives control of the ratio

$$\frac{K(X\setminus Y)}{K(X)} = \mathrm{exp}(-\sum_{M(I(Y))>0} \frac{c(M)}{M!} \prod_{Z\subset X} C(Z)^{M(Z)}).$$

This is just what is needed to analyze measures on spaces of very large dimension.