Trees, functional inversion, and the virial expansion

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Outline

1. Inversion? Trees? Virial expansion?
2. Why not use an inverse function theorem in Banach spaces?
3. An abstract inversion theorem
4. Application in statistical mechanics

Inversion of power series / complex analysis & algebra

Given: a power series in $\mathbb{C}$ of the form

$$f(z) = z + \sum_{n=2}^{\infty} a_n z^n,$$

positive radius of convergence $R(f)$.

Wanted: inverse power series

$$w = f(z) \Leftrightarrow z = g(w) = w + \sum_{n=2}^{\infty} b_n w^n.$$

Questions:

- Is the radius of convergence of the inverse series positive? Holomorphic inverse function theorem.
- Quantitative bounds on $R(g)$? Bloch radii.
- Formulas? Lagrange inversion.
  Also: *The tree formulas for the reversion of power series*, Wright '89, Journal of Pure and Applied Algebra, derived from Abhyankar-Gurjar inversion formula.

What about functionals in infinite-dimensional spaces?
E.g. background potential $\exp(-V_{\mathrm{ext}}(x)) \mapsto$ density profile $\rho(x)$.

Cayley's theorem: number of rooted labelled trees on n vertices

$$t_n = \#\mathcal{T}_n^\bullet = n^{n-1}.$$

Exponential generating function

$$T(z) = \sum_{n=1}^{\infty} \frac{\#\mathcal{T}_n^\bullet}{n!} z^n = \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} z^n \quad \Big(|z| < \frac{1}{\mathrm{e}}\Big).$$

Recursive structure of combinatorial species of trees
$\Rightarrow$ functional equation for generating function:

$$T(z) = z\,\mathrm{e}^{T(z)} = z\left(1 + \sum_{k=1}^{\infty} \frac{1}{k!} T(z)^k\right)$$

Think k = number of children of the root.

Related: $W(z) = -T(-z)$ *Lambert's W-function* solves $z = W \exp(W)$.

Observation:

$$\boxed{z = T(z)\,\mathrm{e}^{-T(z)}, \qquad \frac{1}{\mathrm{e}} = \sup_{x \geq 0} x\,\mathrm{e}^{-x}.}$$

Relation functional equation $\leftrightarrow$ radius of convergence.

Virial expansion / thermodynamics & statistical mechanics

Ideal gas law $pV = Nk_B T$

- p pressure
- V volume
- N number of particles
- k_B Boltzmann constant
- T absolute temperature (in Kelvin, $0\text{ K} = -273.15^\circ\text{ C}$).

Virial expansion: corrections as power series in the density $\rho = N/V$

$$\frac{p}{k_B T} = \rho\Big(1 + C_1\rho + C_2\rho^2 + \cdots\Big).$$

Mayer expansion: series in dual parameter z activity, fugacity

$$\frac{p}{k_B T} = z + B_2 z^2 + B_3 z^3 + \cdots$$

Known:

$$\rho = z\frac{\partial}{\partial z}\frac{p}{k_B T} = z\big(1 + 2B_2 z + 3B_3 z^2 + \cdots\big).$$

From Mayer to virial via inversion $\rho = \rho(z) \Leftrightarrow z = z(\rho)$ Lebowitz, Penrose '64.
What about inhomogeneous systems and position-dependent $z(x)$, $\rho(x)$?

Virial expansion vs. virial theorem

Latin *vis* = "force". ODE for motion of N particles of mass m subject to forces f_i: $m\ddot{x}_i = f_i$. Scalar product with x_i & summation over i $\Rightarrow$

$$-\frac{1}{2}\sum_{i=1}^{N} m x_i \cdot \ddot{x}_i = -\frac{1}{2}\sum_{i=1}^{N} x_i \cdot f_i =: \frac{1}{2} C(\boldsymbol{x})$$

virial of the forces. Integrate over long time intervals, integrate by parts on the left side $\Rightarrow$ long-time averages $\langle\cdot\rangle$ satisfy

$$\left\langle \sum_{i=1}^{N} \frac{1}{2} m \dot{x}_i^2 \right\rangle = \frac{1}{2}\langle C\rangle. \tag{1}$$

Time-average kinetic energy $\leftrightarrow$ time-average of the virial. External forces due to container wall $\rightarrow$ external virial

$$C_{\mathrm{ext}} = 3pV \tag{2}$$

V volume, p pressure. (1) + (2) Clausius virial theorem. Kinetic gas theory:

$$\left\langle \sum_{i=1}^{N} \frac{1}{2} m \dot{x}_i^2 \right\rangle = \frac{3}{2} N k_B T$$

k_B Boltzmann constant, T absolute temperature (in Kelvin). Combine:

$$\boxed{pV = N k_B T - \frac{1}{3}\langle C_{\mathrm{int}}\rangle}$$

Corrections to ideal gas law $\leftrightarrow$ average internal virial.

The trouble with infinite dimensions: a toy example

Countably many variables, map

$$f : \mathbb{C}^{\mathbb{N}} \to \mathbb{C}^{\mathbb{N}}, \quad (z_k)_{k\in\mathbb{N}} \mapsto (\rho_k)_{k\in\mathbb{N}}$$

with

$$\boxed{\rho_1 = z_1, \qquad \forall k \geq 2: \ \rho_k = z_k \, \mathrm{e}^{-kz_1}.}$$

Clearly, invertible. Formally, Jacobian = identity matrix

$$\boxed{\frac{\partial \rho_k}{\partial z_j}(\mathbf{0}) = \delta_{jk}.}$$

Analytic framework? Inverse function theorem? Banach spaces

$$E_a := \Big\{ (z_k)_{k\in\mathbb{N}} \in \mathbb{C}^{\mathbb{N}} : \sum_{k=1}^{\infty} |z_k| \, \mathrm{e}^{ak} < \infty \Big\}, \quad a \in \mathbb{R}.$$

Wanted:
$f : U \to V$ bijection from open neighborhoods of origin $U \subset E_a$ onto $V \subset E_b$.
$f : E_a \supset U \to E_b$ Fréchet-differentiable,
$\mathrm{D}f(\mathbf{0}) : E_a \to E_b$ invertible with bounded inverse.

Problem:
There is no way to choose a and b to make it work.

Proper analytic structure:
scale of Banach spaces, Nash-Moser theorem...

An abstract inversion theorem

Given: formal power series

$$A(q;z) = \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} A_n(q;x_1,\ldots,x_n) z^n(\mathrm{d}\boldsymbol{x}),$$

$A_n : \mathbb{X} \times \mathbb{X}^n \to \mathbb{R}$. Domain of absolute convergence: $z \in \mathscr{D}(A)$ iff

$$\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} \big|A_n(q;x_1,\ldots,x_n)\big| \, |z|^n(\mathrm{d}\boldsymbol{x}) < \infty$$

for all q. Measure-valued map

$$\boxed{\mathscr{D}(A) \ni z \mapsto \rho[z], \quad \rho[z](\mathrm{d}q) = z(\mathrm{d}q)\, \mathrm{e}^{-A(q;z)}.}$$

Wanted: inverse map

$$\rho[z] = \rho \;\Leftrightarrow\; z = z[\rho] \;?$$

Idea:

$$\rho(\mathrm{d}q) = z(\mathrm{d}q)\mathrm{e}^{-A(q;z)} \;\Rightarrow\; z(\mathrm{d}q) = \mathrm{e}^{A(q;z)}\rho(\mathrm{d}q)$$

Thus

$$\boxed{z(\mathrm{d}q) = T_q^{\circ}(\rho)\,\rho(\mathrm{d}q)}$$

with

$$\boxed{T_q^{\circ}(\rho) = \exp\left(\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n} A_n(q;x_1,\ldots,x_n)\,T_{x_1}^{\circ}(\rho)\cdots T_{x_n}^{\circ}(\rho)\rho^n(\mathrm{d}\boldsymbol{x})\right).}$$

Lemma: Fixed point equation determines formal power series

$$T_q^{\circ}(\rho) = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n} t_{n+1}(q,x_1,\ldots,x_n)\rho^n(\mathrm{d}\boldsymbol{x})$$

uniquely.

Proposition:
Coefficients t_n can be expressed as sums over weighted trees.
Generalizes similar relation for finitely many variables from Gessel '87
A combinatorial proof of the multi-variate Lagrange-Good inversion formula.

Formal inversion always possible, inverse expressed with fixed point equation / trees.
Convergence?

Theorem (J, Kuna, Tsagkarogiannis '19)

Suppose that for some $b : \mathbb{X}^n \to \mathbb{R}_+$ *and all* $q \in \mathbb{X}$,

$$\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} \left| A_n(q; x_1, \dots, x_n) \right| \mathrm{e}^{b(x_1)+\dots+b(x_n)} |\rho|^n (\mathrm{d}\boldsymbol{x}) \leq b(q). \qquad (\mathcal{S}_\mathrm{b})$$

Then

$$\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} \left| t_{n+1}(q, x_1, \dots, x_n) \right| \left| \rho \right|^n (\mathrm{d}\boldsymbol{x}) \leq \mathrm{e}^{b(q)} - 1.$$

Theorem (JKT '19)

Fix b *and let* $\mathscr{V}_\mathrm{b}$ *be the set of measures* $\rho(\mathrm{d}q)$ *that satisfy* $(\mathcal{S}_\mathrm{b})$. *Then* $z \mapsto \rho[z]$ *is a bijection from some set* $\mathscr{U}_\mathrm{b}$ *onto* $\mathscr{V}_b$, *and*

$$\rho[z] = \rho \iff z(\mathrm{d}q) = \rho(\mathrm{d}q)\, T_q^\circ(\rho).$$

Considerably improves on J.,Tate,Tsagkarogiannis, Ueltschi '14 where we treated countable spaces $\mathbb{X}$ only.

Application to statistical mechanics

- Box $\Lambda = [0, L]^d$
- pair potential $V(x, y)$
- $\beta = 1/k_B T$ inverse temperature
- measure $z(\mathrm{d}\boldsymbol{x})$, e.g.,

$$z(\mathrm{d}x) = z_0 \exp(-\beta V_{\mathrm{ext}}(x))\mathrm{d}x$$

- Grand-canonical partition function

$$\Xi_\Lambda(z) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} \mathrm{e}^{-\beta \sum_{1 \le i < j \le n} V(x_i, x_j)} z^n(\mathrm{d}\boldsymbol{x}).$$

- Density in the grand-canonical ensemble

$$\int_\Lambda g(x)\rho(\mathrm{d}x) = \frac{1}{\Xi_\Lambda(z)} \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} \left(\sum_{i=1}^{n} g(x_i) \right) \mathrm{e}^{-\beta \sum_{1 \le i < j \le n} V(x_i, x_j)} z^n(\mathrm{d}\boldsymbol{x})$$

for all non-negative test functions g. Admit expansion

$$\boxed{\rho(\mathrm{d}q) = z(\mathrm{d}q) \left(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} \varphi_{n+1}^{\mathsf{T}}(q, x_1, \dots, x_n) z^n(\mathrm{d}\boldsymbol{x}) \right)}.$$

φ_n^{T} Ursell functions, given as sums over connected graphs.

The inverse problem in statistical mechanics

Activity $z(\mathrm{d}x) = z_0 \exp(-\beta V_{\mathrm{ext}}(x))\mathrm{d}x$, density

$$\rho(\mathrm{d}q) = z(\mathrm{d}q)\Big(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} \varphi^{\mathsf{T}}_{n+1}(q, x_1, \dots, x_n) z^n(\mathrm{d}\boldsymbol{x})\Big).$$

Formal inverse well-known Stell, Hiroike-Morita, Evans...

$$z(\mathrm{d}q) = \rho(\mathrm{d}q) \exp\Big(-\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} D_{n+1}(q, x_1, \dots, x_n) \rho^n(\mathrm{d}\boldsymbol{x})\Big)$$

D_{n+1} given as sum over 2-connected graphs.

Question: Can we find V_{ext} so that the density profile associated with V_{ext} equals a given density profile? Chayes, Chayes, Lieb '84

Theorem (JKT '19)

Suppose $V \geq 0$. Let $\rho(x)\mathrm{d}x$ be a density profile such that

$$\int_{\mathbb{R}^d} \big(1 - \mathrm{e}^{-\beta V(x,y)}\big) \mathrm{e}^{a(y)+b(y)} \rho(y)\mathrm{d}y \leq a(x)$$

for some functions $a, b : \mathbb{R}^d \to \mathbb{R}_+$ with $a \leq b$ pointwise. Then

$$\boxed{\beta V_{\mathrm{ext}}(q) = \log z_0 - \log \rho(q) + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\Lambda^n} D_{n+1}(q, x_1, \dots, x_n) \rho(x_1) \cdots \rho(x_n) \mathrm{d}^n \boldsymbol{x}}$$

solves the problem, series is absolutely convergent.

Summary

- We have proven an inversion theorem for maps $z \mapsto \rho$ in measure spaces of the form
$$\rho(\mathrm{d}q) = z(\mathrm{d}q)\mathrm{e}^{-A(q;z)},$$
$A(q;z)$ power series in z.
- **Proof**:
invert on formal level first, then read off convergence condition for formal inverse from fixed point equation (proof by induction).
Philosophy fixed points↔trees↔convergence conditions:
Fernández, Procacci '07, Faris '10.
- When applied to the virial expansion, yields a convergence condition of Kotecký-Preiss type for 2-connected graphs.

Outlook:
Application to other examples?
Connection with other tree formulas?

Gallavotti-Niccoló trees in renormalization group theory—trees for the Lindstedt series in KAM theory—trees for a quantum field theory take on Lagrange-Good inversion Abdesselam—*Butcher trees in numerics...*