Computation of minors and eigenvectors of banded Toeplitz matrices via skew Schur polynomials

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Contents

Toeplitz matrices

$$\begin{bmatrix} a_0 & a_{-1} & a_{-2} & a_{-3} & a_{-4} & a_{-5} \\ a_1 & a_0 & a_{-1} & a_{-2} & a_{-3} & a_{-4} \\ a_2 & a_1 & a_0 & a_{-1} & a_{-2} & a_{-3} \\ a_3 & a_2 & a_1 & a_0 & a_{-1} & a_{-2} \\ a_4 & a_3 & a_2 & a_1 & a_0 & a_{-1} \\ a_5 & a_4 & a_3 & a_2 & a_1 & a_0 \end{bmatrix}.$$

Toeplitz matrices

$$\begin{bmatrix} a_0 & a_{-1} & a_{-2} & a_{-3} & a_{-4} & a_{-5} \\ a_1 & a_0 & a_{-1} & a_{-2} & a_{-3} & a_{-4} \\ a_2 & a_1 & a_0 & a_{-1} & a_{-2} & a_{-3} \\ a_3 & a_2 & a_1 & a_0 & a_{-1} & a_{-2} \\ a_4 & a_3 & a_2 & a_1 & a_0 & a_{-1} \\ a_5 & a_4 & a_3 & a_2 & a_1 & a_0 \end{bmatrix}.$$

Toeplitz matrices are matrices of the form $\left[a_{j-k}\right]_{j,k=1}^{n}$, where $a_{-n+1}, \ldots, a_0, \ldots, a_{n-1}$ are some numbers.

Banded Toeplitz matrices

$$\begin{bmatrix} a_0 & a_{-1} & 0 & 0 & 0 & 0 \\ a_1 & a_0 & a_{-1} & 0 & 0 & 0 \\ a_2 & a_1 & a_0 & a_{-1} & 0 & 0 \\ 0 & a_2 & a_1 & a_0 & a_{-1} & 0 \\ 0 & 0 & a_2 & a_1 & a_0 & a_{-1} \\ 0 & 0 & 0 & a_2 & a_1 & a_0 \end{bmatrix}.$$

Banded Toeplitz matrices

$$\begin{bmatrix} a_0 & a_{-1} & 0 & 0 & 0 & 0 \\ a_1 & a_0 & a_{-1} & 0 & 0 & 0 \\ a_2 & a_1 & a_0 & a_{-1} & 0 & 0 \\ 0 & a_2 & a_1 & a_0 & a_{-1} & 0 \\ 0 & 0 & a_2 & a_1 & a_0 & a_{-1} \\ 0 & 0 & 0 & a_2 & a_1 & a_0 \end{bmatrix}.$$

Laurent polynomial with coefficients a_k: $\qquad a(t) = \sum_{k=-q}^{p} a_k t^k.$

Banded Toeplitz matrices

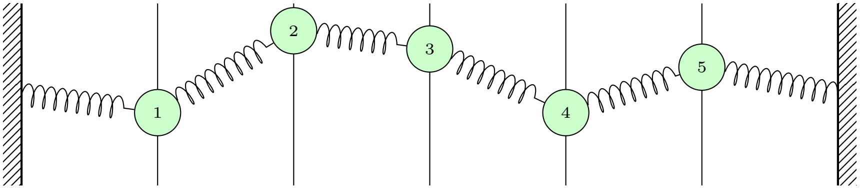
$$T_6(a) = \begin{bmatrix} a_0 & a_{-1} & 0 & 0 & 0 & 0 \\ a_1 & a_0 & a_{-1} & 0 & 0 & 0 \\ a_2 & a_1 & a_0 & a_{-1} & 0 & 0 \\ 0 & a_2 & a_1 & a_0 & a_{-1} & 0 \\ 0 & 0 & a_2 & a_1 & a_0 & a_{-1} \\ 0 & 0 & 0 & a_2 & a_1 & a_0 \end{bmatrix}.$$

Laurent polynomial with coefficients a_k: $\qquad a(t) = \sum_{k=-q}^{p} a_k t^k.$

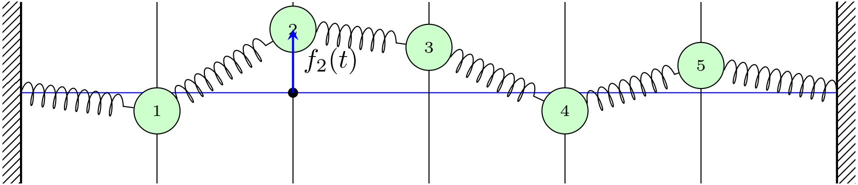
Symmetric real banded Toeplitz matrices

$$\begin{bmatrix} a_0 & a_1 & a_2 & 0 & 0 & 0 \\ a_1 & a_0 & a_1 & a_2 & 0 & 0 \\ a_2 & a_1 & a_0 & a_1 & a_2 & 0 \\ 0 & a_2 & a_1 & a_0 & a_1 & a_2 \\ 0 & 0 & a_2 & a_1 & a_0 & a_1 \\ 0 & 0 & 0 & a_2 & a_1 & a_0 \end{bmatrix}.$$

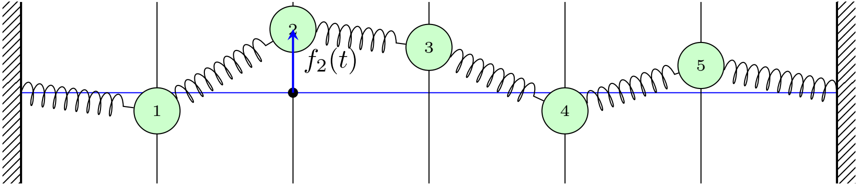
Idea of applications: interactions in homogeneous models



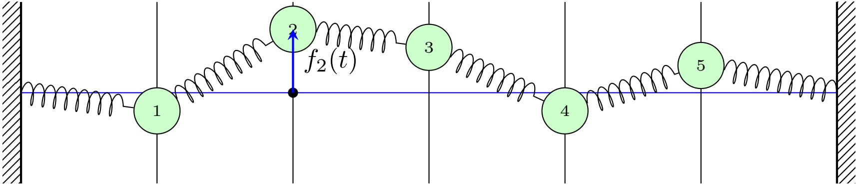
Idea of applications: interactions in homogeneous models



Idea of applications: interactions in homogeneous models



Idea of applications: interactions in homogeneous models



System of differential equations:

$$f_j''(t) = -c^2(-f_{j-1}(t) + 2f_j(t) - f_{j+1}(t)).$$

System of differential equations with Toeplitz matrix

$$f_j''(t) = -c^2(-f_{j-1}(t) + 2f_j(t) - f_{j+1}(t)).$$

$$\begin{bmatrix} f_1''(t) \\ f_2''(t) \\ f_3''(t) \\ f_4''(t) \\ f_5''(t) \end{bmatrix} = -c^2 \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} f_1(t) \\ f_2(t) \\ f_3(t) \\ f_4(t) \\ f_5(t) \end{bmatrix}.$$

$$f''(t) = -c^2 T_n f(t).$$

Some applications of Toeplitz matrices

- The “repeat space theory” (RST) in theoretical chemistry (zero-point vibrational energies of hydrocarbons).
- Ising model of ferromagnetism in statistical quantum mechanics.
- Covariance matrices of stationary stochastic processes.
- Numerical solution of some differential equations.

Contents

Elementary symmetric polynomials

$$\mathrm{e}_0(x_1, x_2) = 1,$$

$$\mathrm{e}_1(x_1, x_2) = x_1 + x_2,$$

$$\mathrm{e}_2(x_1, x_2) = x_1 x_2,$$

$$\mathrm{e}_3(x_1, x_2) = 0,$$

$$\mathrm{e}_4(x_1, x_2) = 0,$$

$$\ldots$$

Elementary symmetric polynomials

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$$\mathrm{e}_3(x_1, x_2) = 0,$$
$$\mathrm{e}_4(x_1, x_2) = 0,$$
$$\ldots$$

$$\mathrm{e}_0(x_1, x_2, x_3) = 1,$$
$$\mathrm{e}_1(x_1, x_2, x_3) = x_1 + x_2 + x_3,$$
$$\mathrm{e}_2(x_1, x_2, x_3) = x_1 x_2 + x_1 x_3 + x_2 x_3,$$
$$\mathrm{e}_3(x_1, x_2, x_3) = x_1 x_2 x_3,$$
$$\mathrm{e}_4(x_1, x_2, x_3) = 0,$$
$$\ldots$$

Elementary symmetric polynomials

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$$\ldots$$

$$\mathrm{e}_0(x_1,x_2,x_3)=1,$$
$$\mathrm{e}_1(x_1,x_2,x_3)=x_1+x_2+x_3,$$
$$\mathrm{e}_2(x_1,x_2,x_3)=x_1x_2+x_1x_3+x_2x_3,$$
$$\mathrm{e}_3(x_1,x_2,x_3)=x_1x_2x_3,$$
$$\mathrm{e}_4(x_1,x_2,x_3)=0,$$
$$\ldots$$

$$\mathrm{e}_m(x_1,\ldots,x_n)=\sum_{1\le k_1<k_2<\ldots<k_m\le n} x_{k_1}x_{k_2}\cdots x_{k_m}.$$

Vieta formula, particular cases

Polynomials of degree 2:

$$\begin{aligned}(t-x_1)(t-x_2) &= t^2-(x_1+x_2)t+x_1x_2\\ &= t^2-\mathrm{e}_1(x_1,x_2)t+\mathrm{e}_2(x_1,x_2).\end{aligned}$$

Vieta formula, particular cases

Polynomials of degree 2:

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Polynomials of degree 3:

$$\begin{aligned}(t-x_1)(t-x_2)(t-x_3) &= t^3-(x_1+x_2+x_3)t^2+(x_1x_2+x_1x_3+x_2x_3)t-x_1x_2x_3\\ &= t^3-\mathrm{e}_1(x_1,x_2,x_3)t^2+\mathrm{e}_2(x_1,x_2,x_3)t-\mathrm{e}_3(x_1,x_2,x_3).\end{aligned}$$

Vieta formula

$$\prod_{k=1}^{n}(t-x_k)=\sum_{k=0}^{n}(-1)^k\,\mathrm{e}_k(x_1,\ldots,x_n)t^{n-k}.$$

Vieta formula

$$\prod_{k=1}^{n}(t - x_k) = \sum_{k=0}^{n}(-1)^k \, \mathrm{e}_k(x_1, \ldots, x_n) t^{n-k}.$$

The coefficients of a univariate polynomial with zeros $x_1, \ldots, x_n$ are symmetric polynomials in $x_1, \ldots, x_n$, with alternating signs.

Complete homogeneous polynomials

$$\mathrm{h}_0(x_1, x_2) = 1,$$

$$\mathrm{h}_1(x_1, x_2) = x_1 + x_2,$$

$$\mathrm{h}_2(x_1, x_2) = x_1^2 + x_1 x_2 + x_2^2,$$

$$\mathrm{h}_3(x_1, x_2) = x_1^3 + x_1^2 x_2 + x_1 x_2^2 + x_2^3,$$

$$\ldots$$

Complete homogeneous polynomials

$$
\begin{aligned}
\mathrm{h}_0(x_1,x_2) &= 1,\\
\mathrm{h}_1(x_1,x_2) &= x_1+x_2,\\
\mathrm{h}_2(x_1,x_2) &= x_1^2+x_1x_2+x_2^2,\\
\mathrm{h}_3(x_1,x_2) &= x_1^3+x_1^2x_2+x_1x_2^2+x_2^3,\\
&\dots
\end{aligned}
$$

$$
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\mathrm{h}_0(x_1,x_2,x_3) &= 1,\\
\mathrm{h}_1(x_1,x_2,x_3) &= x_1+x_2+x_3,\\
\mathrm{h}_2(x_1,x_2,x_3) &= x_1^2+x_1x_2+x_1x_3\\
&\quad +x_2^2+x_2x_3+x_3^2,\\
&\dots
\end{aligned}
$$

Complete homogeneous polynomials

$$\mathrm{h}_0(x_1, x_2) = 1,$$
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$$\mathrm{h}_2(x_1, x_2) = x_1^2 + x_1 x_2 + x_2^2,$$
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$$\mathrm{h}_0(x_1, x_2, x_3) = 1,$$
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$$\mathrm{h}_2(x_1, x_2, x_3) = x_1^2 + x_1 x_2 + x_1 x_3 + x_2^2 + x_2 x_3 + x_3^2,$$
$$\ldots$$

$$\mathrm{h}_m(x_1, \ldots, x_n) = \sum_{p_1 + p_2 + \cdots + p_n = m} x_1^{p_1} x_2^{p_2} \cdots x_n^{p_n}.$$

Computation of complete homogeneous polynomials

Efficient formula for large m:

$$\mathrm{h}_m(x_1,\ldots,x_n)=\sum_{j=1}^{n}\frac{x_j^{n+m-1}}{\prod\limits_{\substack{1\le k\le n\\ k\ne j}}(x_j-x_k)}.$$

Computation of complete homogeneous polynomials

Efficient formula for large m:

$$\mathrm{h}_m(x_1,\ldots,x_n) = \sum_{j=1}^{n} \frac{x_j^{n+m-1}}{\prod\limits_{\substack{1\le k\le n\\ k\ne j}} (x_j - x_k)}.$$

For $n = 3$,

$$\mathrm{h}_m(x_1,x_2,x_3) = \frac{x_1^{m+2}}{(x_1-x_2)(x_1-x_3)} + \frac{x_2^{m+2}}{(x_2-x_1)(x_2-x_1)} + \frac{x_3^{m+2}}{(x_3-x_1)(x_3-x_2)}.$$

Computation of the differences

We want to compute the differences

$$\prod_{\substack{1\le k\le n\\ k\ne j}} (x_j - x_k) \qquad (1 \le j \le n).$$

Idea for an efficient program in Matlab or GNU Octave:

$$\begin{bmatrix} x_1 & x_2 & x_3 \\ x_1 & x_2 & x_3 \\ x_1 & x_2 & x_3 \end{bmatrix} - \begin{bmatrix} x_1 & x_1 & x_1 \\ x_2 & x_2 & x_2 \\ x_3 & x_3 & x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & x_2 - x_1 & x_3 - x_1 \\ x_1 - x_2 & 1 & x_3 - x_2 \\ x_1 - x_3 & x_2 - x_3 & 1 \end{bmatrix}.$$

After that, Octave can just multiply the elements in each column.

$$\begin{bmatrix} x_1 & x_2 & x_3 \\ x_1 & x_2 & x_3 \\ x_1 & x_2 & x_3 \end{bmatrix} - \begin{bmatrix} x_1 & x_1 & x_1 \\ x_2 & x_2 & x_2 \\ x_3 & x_3 & x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & x_2 - x_1 & x_3 - x_1 \\ x_1 - x_2 & 1 & x_3 - x_2 \\ x_1 - x_3 & x_2 - x_3 & 1 \end{bmatrix}.$$

```
function [result] = prod_diffs(x),
    n = length(x);
    xrows = repmat(transpose(x), n, 1);
    xcols = repmat(x, 1, n);
    xdiffs = xrows - xcols + eye(n);
    result = transpose(prod(xdiffs));
end
```

Efficient computation of complete homogeneous polynomials

$$\mathrm{h}_m(x_1,\ldots,x_n) = \sum_{j=1}^{n} \frac{x_j^{n+m-1}}{\prod\limits_{\substack{1\le k\le n\\ k\ne j}} (x_j - x_k)}.$$

```
function [result] = complete_pol(x, m),
    n = length(x); p = n + m + 1;
    numerators = x .^ (p * ones(n, 1));
    denominators = prod_diffs(x);
    result = sum(numerators ./ denominators);
end
```

Contents

Schur polynomials

Let $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_p)$ be an integer partition: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$.

Schur polynomials

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Definition of Schur polynomials by the Jacobi–Trudi formula:

$$\mathrm{s}_\lambda(x_1, \ldots, x_n) = \det\left[\mathrm{h}_{\lambda_j - j + k}(x_1, \ldots, x_n)\right]_{j,k=1}^{p}.$$

Schur polynomials

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For $\lambda = (\lambda_1, \lambda_2, \lambda_3)$,

$$\mathrm{s}_{(\lambda_1,\lambda_2,\lambda_3)}(x_1, \ldots, x_n) = \det \begin{bmatrix} \mathrm{h}_{\lambda_1}(x) & \mathrm{h}_{\lambda_1+1}(x) & \mathrm{h}_{\lambda_1+2}(x) \\ \mathrm{h}_{\lambda_2-1}(x) & \mathrm{h}_{\lambda_2}(x) & \mathrm{h}_{\lambda_2+1}(x) \\ \mathrm{h}_{\lambda_3-2}(x) & \mathrm{h}_{\lambda_3-1}(x) & \mathrm{h}_{\lambda_3}(x) \end{bmatrix}.$$

Schur polynomials

Example.

$$
\begin{aligned}
\mathrm{s}_{(3,1)}(x_1, x_2) &= \det \begin{bmatrix} \mathrm{h}_3(x_1, x_2) & \mathrm{h}_4(x_1, x_2) \\ \mathrm{h}_0(x_1, x_2) & \mathrm{h}_1(x_1, x_2) \end{bmatrix} \\
&= (x_1^3 + x_1^2 x_2 + x_1 x_2^2 + x_2^3)(x_1 + x_2) \\
&\qquad - (x_1^4 + x_1^3 x_2 + x_1^2 x_2^2 + x_1 x_2^3 + x_2^4) \\
&= x_1^3 x_2 + x_1^2 x_2^2 + x_1 x_2^3.
\end{aligned}
$$

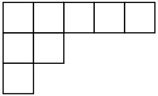
Computation of Schur polynomials

```
function [result] = schur_pol(x, lambda),
    p = length(lambda);
    JT = zeros(p, p);
    for j = 1 : p,
        for k = 1 : p,
            d = lambda(j) - j + k;
            JT(j, k) = complete_pol(x, d);
        end
    end
    result = det(JT);
end
```

Conjugate partition

It is useful to identify integer partitions with Young diagrams:

$$(5, 2, 1) =$$



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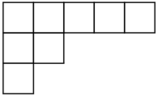
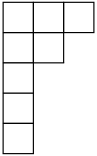


Then, the conjugate partition can be defined via the transposed diagram:

$$(5,2,1)' =$$



$$= (3,2,1,1,1).$$

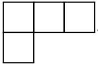
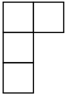
Dual Jacobi–Trudi formula

$$s_\lambda(x_1, \ldots, x_n) = \det\left[e_{\lambda'_j - j + k}(x_1, \ldots, x_n)\right]_{j,k=1}^{\lambda_1}.$$

Dual Jacobi–Trudi formula

$$\mathrm{s}_\lambda(x_1,\ldots,x_n) = \det\big[\mathrm{e}_{\lambda'_j - j + k}(x_1,\ldots,x_n)\big]_{j,k=1}^{\lambda_1}.$$

Example:

$(3,1) =$  , $\qquad (3,1)' =$  $= (2,1,1).$

$$\mathrm{s}_{(3,1)}(x_1,x_2) = \det\begin{bmatrix} \mathrm{e}_2(x_1,x_2) & \mathrm{e}_3(x_1,x_2) & \mathrm{e}_4(x_1,x_2) \\ \mathrm{e}_0(x_1,x_2) & \mathrm{e}_1(x_1,x_2) & \mathrm{e}_2(x_1,x_2) \\ \mathrm{e}_{-1}(x_1,x_2) & \mathrm{e}_0(x_1,x_2) & \mathrm{e}_1(x_1,x_2) \end{bmatrix} = x_1^3 x_2 + x_1^2 x_2^2 + x_1 x_2^3.$$

Skew Schur polynomials

Given a pair of partitions (a so-called "skew partition") λ/μ,

$$\mathrm{s}_{\lambda/\mu}(x_1,\ldots,x_n) := \det\left[\mathrm{h}_{\lambda_j-\mu_k-j+k}(x_1,\ldots,x_n)\right]_{j,k=1}^{p}.$$

Skew Schur polynomials

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Dual Jacobi–Trudi formula:

$$\mathrm{s}_{\lambda/\mu}(x_1,\ldots,x_n) := \det\left[\mathrm{e}_{\lambda'_j-\mu'_k-j+k}(x_1,\ldots,x_n)\right]_{j,k=1}^{\lambda_1}.$$

Contents

Coefficients of a Laurent polynomial as elem. symm. polynomials

$$a(t) = a_2 t^2 + a_1 t^1 + a_0 t^0 + a_{-1} t^{-1}$$
$$= a_2 (t - x_1)(t - x_2)(t - x_3).$$

By Vieta formula,

$$a_1 = -a_2 \, \mathrm{e}_1(x_1, x_2, x_3)$$
$$a_0 = a_2 \, \mathrm{e}_2(x_1, x_2, x_3)$$
$$a_{-1} = -a_2 \, \mathrm{e}_2(x_1, x_2, x_3).$$

Entries of banded Toeplitz matrices as elem. symm. polynomials

$$\begin{bmatrix} a_0 & a_{-1} & 0 & 0 & 0 & 0 \\ a_1 & a_0 & a_{-1} & 0 & 0 & 0 \\ a_2 & a_1 & a_0 & a_{-1} & 0 & 0 \\ 0 & a_2 & a_1 & a_0 & a_{-1} & 0 \\ 0 & 0 & a_2 & a_1 & a_0 & a_{-1} \\ 0 & 0 & 0 & a_2 & a_1 & a_0 \end{bmatrix} = a_2 \begin{bmatrix} \mathrm{e}_2 & -\mathrm{e}_3 & 0 & 0 & 0 & 0 \\ -\mathrm{e}_1 & \mathrm{e}_2 & -\mathrm{e}_3 & 0 & 0 & 0 \\ \mathrm{e}_0 & -\mathrm{e}_1 & \mathrm{e}_2 & -\mathrm{e}_3 & 0 & 0 \\ 0 & \mathrm{e}_0 & -\mathrm{e}_1 & \mathrm{e}_2 & -\mathrm{e}_3 & 0 \\ 0 & 0 & \mathrm{e}_0 & -\mathrm{e}_1 & \mathrm{e}_2 & -\mathrm{e}_3 \\ 0 & 0 & 0 & \mathrm{e}_0 & -\mathrm{e}_1 & \mathrm{e}_2 \end{bmatrix}.$$

After that, the determinants and minors of Toeplitz matrices
can be related with skew Schur polynomials using the dual Jacobi–Trudi formula.

Determinants of banded Toeplitz matrices

If

$$a(t) = \sum_{k=-q}^{p} a_k t^k = a_p (t - x_1) \cdots (t - x_{p+q}),$$

then

$$\det(T_n(a)) = a_p^n (-1)^{pn} \, \mathrm{s}_\lambda(x_1, \ldots, x_{p+q}),$$

where

$$\lambda = (n^p) = (\underbrace{n, \ldots, n}_{p}).$$

The Schur polynomial s_λ is computed as the determinant of $p \times p$ matrix.

The complexity of the formula does not depend on n.

Minors of banded Toeplitz matrices

Consider the Toeplitz matrix $T_n(a)$.
After striking out the rows $\xi_1, \ldots, \xi_d$ and the columns $\eta_1, \ldots, \eta_d$, the determinant of the obtained minor is

$$(-1)^{p(n-d)} a_p^{(n-d)} \, \mathrm{s}_{\lambda/\mu}(x_1, \ldots, x_{p+q}),$$

where

$$\lambda = (\underbrace{n-d, \ldots, n-d}_{p}, \xi_d - d, \ldots, \xi_1 - 1), \qquad \mu = (\eta_d - d, \ldots, \eta_1 - 1).$$

Cofactors of banded Toeplitz matrices

Consider the Toeplitz matrix $T_n(a)$.

The element (r, s) of the adjugated matrix is

$$\operatorname{adj}(T_n(a))_{r,s} = (-1)^{p(n-1)}\, a_p^{n-1}\, \mathrm{s}_{\lambda/\mu}(x_1, \ldots, x_{p+q}),$$

where

$$\lambda = (\underbrace{n-1, \ldots, n-1}_{p}\ s-1), \qquad \mu = (r-1).$$

Eigenvectors of banded Toeplitz matrices

Suppose that λ is an eigenvalue of $T_n(a)$, and

$$a(t) - \lambda = a_p\, t^{-q} \prod_{k=1}^{p+q} (t - x_k).$$

Then the vector $v = [v_r]_{r=1}^{n}$,

$$v_r := \mathrm{s}_{((n-1)^{p-1}, n-r)}(x_1, \ldots, x_{p+q}),$$

is an eigenvector of $T_n(a)$.

Some previous works

- Gabor Szegő (1915),
- Harold Widom (1958),
- Glen Baxter and Palle Schmidt (1961),
- William F. Trench (1985),
- Daniel Bump and Persi Diaconis (2002),
- Per Alexandersson (2012).

Conclusion

The theory of Schur polynomials allows us to pass from determinants or minors of large banded Toeplitz matrices to small determinants of Jacobi–Trudi matrices:

$$\begin{bmatrix} a_0 & a_1 & a_2 & 0 & 0 & 0 \\ a_1 & a_0 & a_1 & a_2 & 0 & 0 \\ a_2 & a_1 & a_0 & a_1 & a_2 & 0 \\ 0 & a_2 & a_1 & a_0 & a_1 & a_2 \\ 0 & 0 & a_2 & a_1 & a_0 & a_1 \\ 0 & 0 & 0 & a_2 & a_1 & a_0 \end{bmatrix} \quad \mapsto \quad \det \begin{bmatrix} \mathrm{h}_n(x_1,x_2) & \mathrm{h}_{n+1}(x_1,x_2) \\ \mathrm{h}_{n-1}(x_1,x_2) & \mathrm{h}_n(x_1,x_2) \end{bmatrix}.$$

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Happy New Year!