

# Stability properties of the Arnoldi Gram-Schmidt process for orthogonal polynomials

Nikos Stylianopoulos University of Cyprus

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#### Bergman polynomials on an archipelago



 $\Gamma_j, j = 1, ..., N$ , a system of disjoint and mutually exterior Jordan curves in  $\mathbb{C}, \overline{G_j := int(\Gamma_j)}, \overline{\Gamma := \cup_{j=1}^N \Gamma_j}, \overline{G := \cup_{j=1}^N G_j}.$ 

$$\langle f,g\rangle := \int_G f(z)\overline{g(z)}dA(z), \quad \|f\|_{L^2(G)} := \langle f,f\rangle^{1/2}$$

The Bergman polynomials  $\{p_n\}_{n=0}^{\infty}$  of *G* are the unique orthonormal polynomials w.r.t. the area measure on *G*:

$$\langle \boldsymbol{p}_m, \boldsymbol{p}_n \rangle = \int_G \boldsymbol{p}_m(z) \overline{\boldsymbol{p}_n(z)} d\boldsymbol{A}(z) = \delta_{m,n},$$

with

$$p_n(z) = \lambda_n z^n + \cdots, \quad \lambda_n > 0, \quad n = 0, 1, 2, \ldots$$



### Construction of the Bergman polynomials

Algorithm: Monomial Gram-Schmidt (GS)

Apply the Gram-Schmidt process to the monomials

$$1, z, z^2, z^3, \ldots$$

Main ingredient: the moments

$$\mu_{m,k} := \langle z^m, z^k \rangle = \int_G z^m \overline{z}^k dA(z), \quad m, k = 0, 1, \dots$$

The above algorithm has been been suggested, and used in practise, by pioneers of Numerical Conformal Mapping, like P. Davis and D. Gaier, in the 1960's, as the standard procedure for constructing Bergman polynomials. It was still treated as the standard method by leaders of the subject, like P. Henrici (*Computational Complex Analysis*, Vols I,II and III), in the 1980's.



### The interior conformal mapping for a single island



In the single island case N = 1, we fix  $z_0 \in G$  and consider the interior conformal mapping:

$$\varphi_{z_0}: G \to \mathbb{D} \quad \text{with} \quad \varphi_{z_0}(z_0) = 0, \quad \text{and} \quad \varphi'_{z0}(z_0) > 0.$$

Computationally, it is easier to approximate the normalized mapping

$$f_0(z) := rac{\varphi_{z0}(z)}{\varphi'_{z0}(z_0)},$$
 so that  $f_0(z_0) = 0$  and  $f'_0(z_0) = 1.$ 



#### Series representation for the Bergman kernel

Let  $K(z, z_0)$  denote the reproducing kernel of the Bergman space  $L^2_a(G)$  w.r.t. the point evaluation at  $z_0$ . Then,

$$\mathcal{K}(z, z_0) = \sum_{j=0}^{\infty} \overline{p_j(z_0)} p_j(z), \quad ext{locally uniformly in } G.$$

The Bergman kernel  $K(\cdot, z_0)$  is related to the mapping function  $f_0$  by

$$f_0(z) = \frac{1}{K(z_0, z_0)} \int_{z_0}^{z} K(\zeta, z_0) d\zeta.$$
 (1)

This relation yields the Bergman kernel method: Construct the Bergman polynomials  $\{p_n\}_{n=0}^n$  of *G* and form the finite Fourier sum

$$K_n(z,z_0)=\sum_{j=0}^n\overline{p_j(z_0)}p_j(z).$$

Then, replace  $K(\zeta, z_0)$  by  $K_n(\zeta, z_0)$  in (1) to approximate  $f_0(z)$ .

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#### Instability Indicator

The GS method is notorious for its instability. For measuring it, when orthonormalizing a system  $S_n := \{u_0, u_1, \dots, u_n\}$  of functions, in a Hilbert space with norm  $\|\cdot\|$ , the following instability indicator has been proposed by J.M. Taylor, (Proc. R.S. Edin., 1978):

$$I_n := rac{\|u_n\|^2}{\min_{u \in \text{span}(S_{n-1})} \|u_n - u\|^2}, \quad n \in \mathbb{N}.$$

Note that, when  $S_n$  is an orthonormal system, then  $\lfloor I_n = 1 \rfloor$ . When  $S_n$  is linearly dependent then  $\lfloor I_n = \infty \rfloor$ . Also, if  $G_n := [\langle u_m, u_k \rangle]_{m,k=0}^n$ , denotes the Gram matrix associated with  $S_n$  then,

$$\kappa(G_n) \geq I_n$$
,

where  $\kappa(G_n) := \|G_n\| \|G_n^{-1}\|$  is the spectral condition number of  $G_n$ .



### Instability of the Monomial GS process: Theory

In the single-component case N = 1, consider the set of monomials  $S_n = \{1, z, z^2, ..., z^n\}$ . Then, for the resulting GS process we have the following result:

Theorem (Papamichael & Warby, Numer. Math., 1986)

Assume that the curve  $\Gamma$  is piecewise-analytic without cusps and let

$$L := \| z \|_{L^{\infty}(\Gamma)} / \operatorname{cap}(\Gamma) | \quad (\geq 1),$$

where  $cap(\Gamma)$  denotes the logarithmic capacity of  $\Gamma$ . Then,

$$c_1(\Gamma) L^{2n} \leq I_n \leq c_2(\Gamma) L^{2n}$$

Note that L = 1, iff  $G \equiv \mathbb{D}_r$  and that  $I_n$  is sensitive to the relative position of *G* w.r.t. the origin. When *G* is the 8 × 2 rectangle centered at the origin, then  $L = 3/\sqrt{2} \approx 2.12$ . In this case,  $I_{25} \approx 10^{16}$  and the method breaks down in MATLAB or FORTRAN, for n = 25.



### Instability of the Monomial GS process: Practise

#### Example (Papamichael & Warby, Numer. Math., 1986)

Ellipse: 
$$G := \{(x, y) : x^2/8^2 + y^2 = 1\}$$

- Optimal max degree in the BKM: n = 7.
- Uniform error estimate:  $1.7 \times 10^{-1}$ .
- Monomial GS breaks down for n = 16.

Computing environment double precision FORTRAN.



## Instability of the Monomial GS process: Practise

#### Example (Papamichael & Warby, Numer. Math., 1986)

L-shaped:

- $G := \{(x,y): -1 < x < 3, |y| < 1\} \cup \{(x,y): |x| < 1, -1 < y < 3\}$ 
  - Optimal max degree in the BKM: *n* = 13.
  - Uniform error estimate:  $2.4 \times 10^{-1}$ .
  - Monomial GS breaks down for n = 26.

Computing environment double precision FORTRAN.



### Instability of the Monomial GS process: Archipelago

As it is expected, things cannot get any better in the archipelago case.

#### Theorem

Let G be an archipelago and consider the application of the GS process to the monomials  $S_n = \{1, z, z^2, ..., z^n\}$ . Assume that boundary  $\Gamma$  of G satisfies an interior cone condition at the point  $z_0$ , where  $|z_0| = ||z||_{L^{\infty}(\Gamma)}$  and let

$$L := \|z\|_{L^{\infty}(\Gamma)} / \operatorname{cap}(\Gamma) \quad (\geq 1).$$

Then

$$c_1(\Gamma) L^{2n} \leq I_n \leq c_2(\Gamma) L^{2n}$$



### The Arnoldi algorithm in Numerical Linear Algebra

Let  $A \in \mathbb{C}^{m,m}$ ,  $b \in \mathbb{C}^m$  and consider the Krylov subspace

$$K_k := \operatorname{span}\{b, Ab, A^2b \dots, A^{k-1}b\},\$$

for solving the system Ax = b. Then, the Arnoldi algorithm (W. Arnoldi , Quart. Appl. Math., 1951) produces an orthonormal basis { $v_1, v_2, ..., v_k$ } of  $K_k$  as follows:

At the *n*-th step, apply GS to orthonormalize the vector  $Av_{n-1}$  (instead of  $A^{n-1}b$ ) against the (already computed) orthonormal vectors  $\{v_1, v_2, \ldots, v_{n-1}\}$ .



### The Arnoldi algorithm for OP's

Let  $\mu$  be a (non-trivial) finite Borel measure with compact support  $supp(\mu)$  on  $\mathbb{C}$  and consider the associated series of orthonormal polynomials

 $p_n(z,\mu) := \lambda_n(\mu) z^n + \cdots, \quad \lambda_n(\mu) > 0, \quad n = 0, 1, 2, \dots,$ 

generated by the inner product

$$\langle f, g \rangle_{\mu} = \int f(z) \overline{g(z)} d\mu(z), \quad \|f\|_{L^{2}(\mu)} := \langle f, g \rangle_{\mu}^{1/2}$$

#### Arnoldi GS for Orthonormal Polynomials

At the *n*-th step, apply GS to orthonormalize the polynomial  $zp_{n-1}$  (instead of  $z^n$ ) against the (already computed) orthonormal polynomials  $\{p_0, p_1, \ldots, p_{n-1}\}$ .

Suggested by Gragg & Reichel (Linear Algebra Appl. (1987)), for the construction of Szegö polynomials, in connection with the search of optimal polynomial iteration methods for solving large linear systems.

Construction Asymptotics Archipelago

Monomial GS Arnoldi GS



## Only ellipses carry short-term recurrences for $p_n$

#### Definition

We say that the polynomials  $\{p_n\}_{n=0}^{\infty}$  satisfy an *M*-term recurrence relation, if for any  $n \ge M$ ,

$$zp_n(z) = a_{n+1,n}p_{n+1}(z) + a_{n,n}p_n(z) + \ldots + a_{n-M,n}p_{n-M}(z).$$

#### Theorem (St, C. R. Acad. Sci. Paris, 2010)

Assume that:

- (i)  $\Gamma = \partial G$  is piecewise analytic without cusps.
- (ii) The Bergman polynomials {p<sub>n</sub>}<sub>n=0</sub><sup>∞</sup> satisfy an M-term recurrence relation, with some M ≥ 3.

Then M = 3 and  $\Gamma$  is an ellipse.

The above theorem refines some deep results of Putinar & St (CAOT, 2007) and Khavinson & St (Springer, 2010).



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## Banded Hessenberg matrices for OP's are Jacobi

In the Numerical Linear Algebra jargon the previous theorem reads as:

#### Corollary

If the Hessenberg matrix associated with the Bergman polynomials  $\{p_n\}$  is banded with constant bandwidth  $\geq$  3, then it is tridiagonal, i.e., a Jacobi matrix.

This result should put an end to the long search in Numerical Linear Algebra, for practical polynomial iteration methods based on short-term recurrence relations of orthogonal polynomials.



### Stability of the Arnoldi GS

In the case of the Arnoldi GS, the instability indicator is given by:

$$I_n = \frac{\|zp_{n-1}\|_{L^2(\mu)}^2}{\min_{p \in \mathbb{P}_{n-1}} \|zp_{n-1} - p\|_{L^2(\mu)}^2}, \quad n \in \mathbb{N}.$$

Theorem (St, Constr. Approx. (accepted))

It holds,

$$1 \leq I_n \leq \|Z\|_{L^{\infty}(\mathrm{supp}(\mu))} \frac{\lambda_n^2(\mu)}{\lambda_{n-1}^2(\mu)}, \quad n \in \mathbb{N}.$$

It turns out that when  $d\mu \equiv |dz|$  (Szegö polynomials), or  $d\mu \equiv dA$  (Bergman polynomials), then

$$oldsymbol{c}_1(\mu) \, \leq \, rac{\lambda_n(\mu)}{\lambda_{n-1}(\mu)} \leq \, oldsymbol{c}_2(\mu) \, , \quad n \in \mathbb{N}.$$

When  $d\mu \equiv w(x)dx$  on  $[a, b] \subset \mathbb{R}$ , this ratio tends to a constant.

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#### Asymptotics: Single-component case N = 1

$$\widehat{\Omega} := \overline{\mathbb{C}} \setminus \overline{\overline{G}}$$

$$\Phi(z) = \gamma z + \gamma_0 + \frac{\gamma_1}{z} + \frac{\gamma_2}{z^2} + \cdots$$

$$\widehat{\Omega} := \overline{\mathbb{C}} \setminus \overline{\mathbb{C}}$$

$$\widehat{\nabla} := \overline{\mathbb{C}} \setminus \overline{\mathbb{C}}$$

The Bergman polynomials of G:

$$p_n(z) = \lambda_n z^n + \cdots, \quad \lambda_n > 0, \quad n = 0, 1, 2, \dots$$



### Strong asymptotics when Γ is analytic



T. Carleman, Ark. Mat. Astr. Fys. (1922)

If  $\rho < 1$  is the smallest index for which  $\Phi$  is conformal in  $ext(L_{\rho})$ , then

$$\frac{n+1}{\pi}\frac{\gamma^{2(n+1)}}{\lambda_n^2} = 1 - \alpha_n \, , \text{ where } 0 \le \alpha_n \le c_1(\Gamma) \, \rho^{2n}$$

$$p_n(z) = \sqrt{rac{n+1}{\pi}} \Phi^n(z) \Phi'(z) \{1 + A_n(z)\}$$
,  $n \in \mathbb{N}$ ,

where

$$|A_n(z)| \leq c_2(\Gamma)\sqrt{n}\,\rho^n, \quad z\in\overline{\Omega}.$$

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#### Strong asymptotics for Γ non-smooth

Theorem (St, C. R. Acad. Sci. Paris, 2010 & Constr. Approx.)

Assume that  $\Gamma$  is piecewise analytic without cusps. Then, for  $n \in \mathbb{N}$ ,

$$\frac{n+1}{\pi}\frac{\gamma^{2(n+1)}}{\lambda_n^2}=1-\alpha_n\,,$$

where 
$$0 \le \alpha_n \le c(\Gamma) \frac{1}{n}$$

and for any  $z \in \Omega$ ,

$$p_n(z) = \sqrt{\frac{n+1}{\pi}} \Phi^n(z) \Phi'(z) \{1 + A_n(z)\}$$

where

$$|A_n(z)| \leq \frac{c_1(\Gamma)}{\operatorname{dist}(z,\Gamma) |\Phi'(z)|} \frac{1}{\sqrt{n}} + c_2(\Gamma) \frac{1}{n}$$

Letting  $z \to \infty$ , we recover the result for the leading coefficients.



### Ratio asymptotics for $\lambda_n$

# Corollary (St, C. R. Acad. Sci. Paris, 2010) $\sqrt{\frac{n+1}{n}} \frac{\lambda_{n-1}}{\lambda_n} = \operatorname{cap}(\Gamma) + \xi_n, \quad \text{where} \quad |\xi_n| \le c(\Gamma) \frac{1}{n}, \quad n \in \mathbb{N}.$

The above relation provides the means for computing approximations to the capacity of  $\Gamma$ , by using only the leading coefficients of the Bergman polynomials. In addition, it implies for the Instability Indicator  $I_n$  of the Arnoldi GS:

#### Corollary

$$c_1(\Gamma) \leq I_n \leq c_2(\Gamma)$$
,  $n \in \mathbb{N}$ .

Hence, the Arnoldi GS for Bergman polynomials, in the single component case, is stable.



## Stability of the Arnoldi GS process: Practise

#### Example (Lytrides & St, CMFT 2011)

Symmetric lens-shaped domain of opening angles  $\pi/2$ .

- BKM with *n* = 35.
- Uniform error estimate:  $1.3 \times 10^{-4}$ .

Computing environment Maple with 16 significant figures.



#### Ratio asymptotics for $p_n(z)$

Corollary (St, C. R. Acad. Sci. Paris, 2010)

For any  $z \in \Omega$ , and sufficiently large  $n \in \mathbb{N}$ ,

$$\sqrt{\frac{n}{n+1}}\frac{p_n(z)}{p_{n-1}(z)}=\Phi(z)\{1+B_n(z)\},$$

where

$$|B_n(z)| \leq \frac{c_1(\Gamma)}{\sqrt{\operatorname{dist}(z,\Gamma)} |\Phi'(z)|} \frac{1}{\sqrt{n}} + c_2(\Gamma) \frac{1}{n}.$$

The above relation, combined with the Arnoldi GS for constructing the Bergman polynomials  $p_n(z)$ , n = 0, 1, ..., provides an efficient method for computing approximations to  $\Phi(z)$ .



### Example: Computing the capacity of a Square

n	$\sqrt{\frac{n+1}{n}} \frac{\lambda_{n-1}}{\lambda_n}$	$\sqrt{rac{n+1}{n}}rac{\lambda_{n-1}}{\lambda_n} - \operatorname{cap}(\Gamma)$	S
100	0.834 640 612	1.37e-05	-
110	0.834 638 233	1.14e-05	1.9902
120	0.834 636 420	9.58e-06	1.9911
130	0.834 635 009	8.16e-06	1.9918
140	0.834 633 888	7.04e-06	1.9924
150	0.834 632 982	6.14e-06	1.9930
160	0.834632341	5.39e-06	1.9934
170	0.834 631 626	4.78e-06	1.9938
180	0.834631111	4.26e-06	1.9942
190	0.834630674	3.83e-06	1.9945
200	0. <mark>834 63</mark> 0 301	3.46e-06	1.9949

Γ: Square with corners at 1, *i*, -1, -i. |cap(Γ) = 0.834626841...

s: tests the hypothesis  $\xi_n = \sqrt{\frac{n+1}{n}} \frac{\lambda_{n-1}}{\lambda_n} - \operatorname{cap}(\Gamma) \approx C \frac{1}{n^s}$ .



### When ratio asymptotics were regarded as useless

The Monomial Gram-Schmidt process was, indeed, a true obstacle back then:

Henrici, Computational Complex Analysis, III (1986)

...However, the construction of a long sequence of orthogonal functions by means of the Gram-Schmidt process may run into difficulties, and the author knows of no nontrivial example where an accurate determination of  $\Phi(z)$  via  $\sqrt{\frac{n}{n+1}} \frac{p_n(z)}{p_{n-1}(z)}$  was actually carried over.



#### Discovery of an archipelago

#### Research in Pairs, Oberwolfach, January 2008



#### Bjorn Gustafsson, Ed Saff, Mihai Putinar

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#### Asymptotics in an archipelago



Let  $g_{\Omega}(z,\infty)$  denote the Green function of  $\Omega := \overline{\mathbb{C}} \setminus \overline{G}$  with pole at  $\infty$ .

Theorem (Gustafsson, Putinar, Saff & St, Adv. Math., 2009)

Assume that every  $\Gamma_i$  is analytic. Then, for  $n \in \mathbb{N}$ :

(i) There exists a positive constant C, so that

$$|p_n(z)| \leq \frac{C}{\operatorname{dist}(z,\Gamma)} \sqrt{n} \exp\{ng_\Omega(z,\infty)\}, \quad z \notin \overline{G}.$$

(ii) For every  $\epsilon > 0$  there exist a constant  $C_{\epsilon} > 0$ , such that

 $|p_n(z)| \ge C_{\epsilon}\sqrt{n}\exp\{ng_{\Omega}(z,\infty)\}, \quad \operatorname{dist}(z,\operatorname{Co}(\overline{G})) \ge \epsilon.$ 

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#### Leading coefficients for an archipelago



Theorem (Gustafsson, Putinar, Saff & St, Adv. Math., 2009) Assume that every  $\Gamma_i$  is analytic, j = 1, 2, ..., N. Then, for  $n \in \mathbb{N}$ ,

$$c_1(\Gamma)\sqrt{rac{n+1}{\pi}}rac{1}{ ext{cap}(\Gamma)^{n+1}} \leq \lambda_n \leq c_2(\Gamma)\sqrt{rac{n+1}{\pi}}rac{1}{ ext{cap}(\Gamma)^{n+1}}.$$

In view of the strong asymptotics in the single island case, this looks a bit disappointing...



### Leading coefficients for a lemniscate

However, the following result shows that we can not expect to do any better, in general, than the previous double inequality.

Theorem (Gustafsson, Putinar, Saff & St, Adv. Math., 2009)

Consider the lemniscate  $G := \{z : |z^m - 1| < r^m\}$ ,  $m \ge 2$ , 0 < r < 1, and note that  $cap(\Gamma) = r$ . Then, the sequence

$$\lambda_n \operatorname{cap}(\Gamma)^{n+1} \sqrt{rac{\pi}{n+1}}, \quad n \in \mathbb{N},$$

has exactly m limit points:

$$\frac{1}{r^{m-1}}, \frac{1}{r^{m-2}}, \ldots, \frac{1}{r}, 1.$$

#### Construction Asymptotics Archipelago

#### Theory Recovery



### A question regarding ratio asymptotics

The important class **Reg** of measures of orthogonality was introduced by Stahl and Totik in *General Ortho Polys*, CUP (1992). Recall that  $\mu \in \text{Reg}$  if

$$\lim_{n\to\infty}\lambda_n^{1/n}(\mu)=\frac{1}{\operatorname{cap}(\Gamma)}$$

Motivated by the crucial properties of the ratio asymptotics outlined above, we have asked the following:

#### Question

Characterize all the measures of orthogonality  $\mu$ , for which it holds:

$$\lim_{n \to \infty} \frac{\lambda_{n+1}(\mu)}{\lambda_n(\mu)} = \frac{1}{\operatorname{cap}(\Gamma)} \quad \text{or} \quad \boxed{c_1 \leq \frac{\lambda_{n+1}(\mu)}{\lambda_n(\mu)} \leq c_2}$$

Clearly, such measures will be in the Reg class.



#### Recovery from area moments

**Truncated Moments Problem** 

Given the finite  $n + 1 \times n + 1$  section  $[\mu_{m,k}]_{m,k=0}^{n}$ ,

$$\mu_{m,k} := \int_G z^m \overline{z}^k dA(z),$$

of the infinite complex moment matrix  $[\mu_{m,k}]_{m,k=0}^{\infty}$ , associated with an archipelago *G*, compute a good approximation to its boundary  $\Gamma$ .

Theorem (Davis & Pollak, Trans. AMS, 1956)

The infinite matrix  $[\mu_{m,k}]_{m,k=0}^{\infty}$  defines uniquely  $\Gamma$ .

This leads to applications in 2D geometric tomography, through the Radon transform.

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#### Discovery of an archipelago



Archipelago Recovery Algorithm Gustafsson, Putinar, Saff & St, Adv. Math., 2009.

- (I) Use the Arnoldi GS to compute  $p_0, p_1, \ldots, p_n$ , from  $[\mu_{m,k}]_{m,k=0}^n$ .
- (II) Form the square root of the Christoffel function

$$\Lambda_n(z) := 1/\sqrt{\sum_{k=0}^n |p_k(z)|^2}.$$

- (III) Plot the zeros of  $p_j$ , j = 1, 2, ..., n.
- (IV) Plot the level curves of the function  $\Lambda_n(x + iy)$ , on a suitable rectangular frame for (x, y) that surrounds the plotted zero set.



#### Three-disks



Theory in: Gustafsson, Putinar, Saff & St, Adv. Math., 2009.

Construction Asymptotics Archipelago

Theory Recovery



#### Recovery of three disks



Level lines of  $\Lambda_n(x + iy)$  on  $\{(x, y) : -1 \le x \le 4, -2 \le y \le 2\}$ , for n = 25, 50, 75, 100.





#### Pentagon and disk



Theory in: Gustafsson, Putinar, Saff & St, Adv. Math., 2009.





Level lines of  $\Lambda_n(x + iy)$  on  $\{(x, y) : -2 \le x \le 5, -2 \le y \le 2\}$ , for n = 25, 50.

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#### Theoretical support of the recovery algorithm



Theorem (Gustafsson, Putinar, Saff & St, Adv. Math., 2009)

Assume that every  $\Gamma_j$  is analytic and let  $\Omega := \overline{\mathbb{C}} \setminus \overline{G}$ . Then,

$$\begin{array}{lll} \Lambda_n(z) &\asymp & {\rm dist}(z,\Gamma), \quad z\in G, \quad n\to\infty\\ \Lambda_n(z) &\asymp & \frac{1}{n}, \quad z\in\Gamma, \quad n\to\infty\\ \Lambda_n(z) &\asymp & \frac{1}{\sqrt{n}}\exp\{-n\,g_\Omega(z,\infty)\}, \quad z\in\Omega, \quad n\to\infty. \end{array}$$

where  $g_{\Omega}(z,\infty)$  denotes the Green function of  $\Omega$  with pole at infinity.

Note:  $g_{\Omega}(z,\infty) > 0, \quad z \in \Omega$ .