Antecedents of the LR algorithm

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Standard Model

- LR [Rutishauser, 1957/58]
- QR [Francis (Kublanovskaja), 1960/1961]
- IEEE/ Amer. Inst. of Physics 2000
  Computing in Science and Engineering
  "Top 10 Algorithms of the Century" (includes QR)
  Jan/Feb 1900-2000
- F. A. Grunbaum [1986]

- 2^{nd} order linear differential operators in Schroedinger form:

$$L = -D^2 + V(x), \qquad D = \frac{d}{dx}$$

- The Darboux transform (1882):

$$V \longrightarrow \tilde{V}$$

- For any $\phi_0 \in \ker(L)$, $L\phi_0 = 0$,

$$\tilde{V} = V - 2\left(\frac{\phi_0'}{\phi_0}\right)' = -V + 2\left(\frac{\phi_0'}{\phi_0}\right)^2$$
$$\tilde{L} = -D^2 + \tilde{V}(x)$$

Example

$$\left.\begin{array}{rl} V_0 & = 0 \\ \ker(L_0) & = \operatorname{span}(1, x) \\ \phi_0(x) & = C(x-t) \end{array}\right\} \Longrightarrow \quad \begin{array}{rl} V_1(x) & = -0 + 2\left(\frac{C}{C(x-t)}\right)^2 \\ & = \frac{1\cdot 2}{(x-t)^2} \end{array},$$

where t is a free parameter.

$$\left.\begin{array}{rl} V_1 & = \frac{2}{(x-t)^2} \\ \ker(L_1) & = \operatorname{span}\left[(x-t_1)^2, \ \frac{1}{(x-t_1)}\right] \\ \phi_1(x) & = (x-t)^2 \end{array}\right\} \Longrightarrow \quad \begin{array}{rl} V_2(x) & = -\frac{2}{(x-t)^2} + 2\left(\frac{2}{(x-t)}\right)^2 \\ & = \frac{2\cdot 3}{(x-t)^2} \end{array}$$

And so on.

$$V_3(x) = \frac{3 \cdot 4}{(x-t)^2}$$

The potential in the Darboux transformation depends on the choice of

$$\phi_0 \in \ker(L)$$

Amazing fact:

All the potentials thus obtained are the potentials that remain rational under the Korteweg-de Vries flow:

$$V_t = V_{xxx} + 6VV_x$$

[Moser and co-workers, 1977/78]

or, equivalently,

$V(\infty)$ finite, eigenfunctions of L are meromorphic in$C$.

Burchnall and Chaundy [1923] (interpret Darboux)

$$L = -D^2 + V(x), \qquad L\phi_0 = 0$$

Define:

$$P = -D - \left(\frac{\phi_0'}{\phi_0}\right), \qquad Q = D - \left(\frac{\phi_0'}{\phi_0}\right)$$

$$
\begin{aligned}
PQ\psi &= -D^2\psi + D\left(\frac{\phi_0'}{\phi_0}\psi\right) - \frac{\phi_0'}{\phi_0}\psi' + \left(\frac{\phi_0'}{\phi_0}\right)^2\psi \\
&= -D^2\psi + D\left(\frac{\phi_0'}{\phi_0}\right)\psi + \left(\frac{\phi_0'}{\phi_0}\right)^2\psi \\
&= -D^2\psi + \left[\left(\frac{\phi_0'}{\phi_0}\right)' + \left(\frac{\phi_0'}{\phi_0}\right)^2\right]\psi \\
&= -D^2\psi + \left(\frac{\phi_0''}{\phi_0}\right)\psi \\
&= L\psi
\end{aligned}
$$

$$\begin{aligned} QP\psi &= -D^2\psi - D\left(\frac{\phi_0'}{\phi_0}\psi\right) + \frac{\phi_0'}{\phi_0}\psi' + \left(\frac{\phi_0'}{\phi_0}\right)^2 \psi \\ &= -D^2\psi - D\left(\frac{\phi_0'}{\phi_0}\right)\psi + \left(\frac{\phi_0'}{\phi_0}\right)^2 \psi \\ &= -D^2\psi + \left[-\left(\frac{\phi_0'}{\phi_0}\right)' + \left(\frac{\phi_0'}{\phi_0}\right)^2\right]\psi \\ &= -D^2\psi + \left[-V + 2\left(\frac{\phi_0'}{\phi_0}\right)^2\right]\psi \\ &= \tilde{L}\psi \end{aligned}$$

$$L\phi = \phi\lambda \Longrightarrow \tilde{L}(Q\phi) = (Q\phi)\lambda, \qquad \lambda \neq 0$$

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The Factorization Method

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The factorization method is an operational procedure which enables us to answer, in a direct manner, questions about eigenvalue problems which are of importance to physicists. The underlying idea is to consider a *pair* of first-order differential-difference equations which are equivalent to a given second-order differential equation with boundary conditions. For a large class of such differential equations the method enables us to find immediately the eigenvalues and a manufacturing process for the normalized eigenfunctions. These results are obtained merely by consulting a table of the six possible factorization types.

The manufacturing process is also used for the calculation of transition probabilities.

The method is generalized so that it will handle perturbation problems.

TABLE OF CONTENTS

Eigenvalue Problems in Mathematical Physics

- PDE
- Separation of variables + Boundary Conditions
- Sequence of ODE's with parameter $m = 0, 1, 2, \ldots$

$$y''(x) + \left[r(x, m) + \lambda\right] y(x) = 0 \qquad (ODE)$$

Eigenvalues: $\lambda_0, \lambda_1, \lambda_2, \ldots \qquad \{\lambda_l\}$

Eigenfunctions: $y_l^m = y(\lambda, m)$, supress x.

Definition

The ODE can be factored if it is equivalent to both

$$\left({}^{+}H^{m+1}\right)\left({}^{-}H^{m+1}\right)y(\lambda, m) = \left[\lambda - L(m+1)\right]y(\lambda, m)$$
$$\left({}^{-}H^{m}\right)\left({}^{+}H^{m}\right)y(\lambda, m) = \left[\lambda - L(m)\right]y(\lambda, m)$$

where

$$^{\pm}H^{m} = k(x, m) \pm \frac{d}{dx} \quad \text{and} \quad L \text{ is independent of } x \text{ and } \lambda.$$

Hence, as differential operators,

$$\left({}^{+}H^{m+1}\right)\left({}^{-}H^{m+1}\right) = \left({}^{-}H^{m}\right)\left({}^{+}H^{m}\right) - \left[L(m+1) - L(m)\right]$$

Noted, in passing, by I&H, but not developed.   Why?

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Try backward and forward difference operators for $\frac{d}{dx}$.

Get LR on a tridiagonal.

Associated Spherical Harmonics:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\,\frac{dP}{d\theta}\right) - \frac{m^2}{\sin^2\theta}P + \lambda P = 0, \quad \theta \in [0,\pi]$$

Standard form:

$$Y(\theta) = \sin^{\frac{1}{2}}\theta\,P(\theta)$$

$$Y'' - \frac{m^2 - \frac{1}{4}}{\sin^2\theta}Y + \left(\lambda + \frac{1}{4}\right)Y = 0, \quad m = 1, 2, \ldots$$

Clever factorizations:

$$\left[\left(m-\tfrac{1}{2}\right)\cot\theta-\frac{d}{d\theta}\right]\left[\left(m-\tfrac{1}{2}\right)\cot\theta-\frac{d}{d\theta}\right]Y$$

$$=\left[\lambda-\left(m-\tfrac{1}{2}\right)^2+\tfrac{1}{4}\right]Y$$

and

$$\left[\left(m+\tfrac{1}{2}\right)\cot\theta-\frac{d}{d\theta}\right]\left[\left(m+\tfrac{1}{2}\right)\cot\theta-\frac{d}{d\theta}\right]Y$$

$$=\left[\lambda-\left(m+\tfrac{1}{2}\right)^2+\tfrac{1}{4}\right]Y$$

17. Table of Factorizations—*Continued*

Name	$r(x, m)$	$k(x, m)$	$L(m)$
Generalized spherical harmonics	$-\frac{(m+\gamma)(m+\gamma-1)}{\sin^2\theta}$	$(m+\gamma-1)\cot\theta$	$(m+\gamma-1)^2$
Generalized spherical harmonics	$\frac{(l+\gamma-\frac{1}{2})(l+\gamma+\frac{1}{2})}{\cosh^2 z}$	$(l+\gamma-\frac{1}{2})\tanh z$	$-(l+\gamma-\frac{1}{2})^2$
Gegenbauer functions	$-\frac{m(m+1)}{\sin^2\theta}$	$m\cot\theta$	m^2
Symmetric top functions	$-\frac{(M-\frac{1}{2})(M+\frac{1}{2})+K^2-2MK\cos\theta}{\sin^2\theta}$	$(M-\frac{1}{2})\cot\theta-\frac{K}{\sin\theta}$	$(M-\frac{1}{2})^2$
Harmonics with spin, magnetic pole	$-\frac{m(m+1)+\frac{1}{4}\pm(m+\frac{1}{2})\cos\theta}{\sin^2\theta}$	$m\cot\theta\pm\frac{1}{2\sin\theta}$	m^2
Pöschl-Teller, hypergeometric	$-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sin^2\rho}$	$(m+c-\frac{3}{2})\cot\rho$	$(2m+a+b-2)^2$
	$-\frac{(m+a+b-c-\frac{1}{2})(m+a+b-c+\frac{1}{2})}{\cos^2\rho}$	$-(m+a+b-c-\frac{1}{2})\tan\rho$	
Pöschl-Teller, hypergeometric	$-\frac{(m+a+b-c-\frac{1}{2})(m+a+b-c+\frac{1}{2})}{\sinh^2 y}$	$(m+a+b-c-\frac{1}{2})\coth y$	$-(2m+2a-c-1)^2$

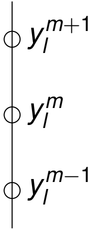
Theorem 1

How factorization works.

$$y(\lambda, m+1) = {}^{-}H^{m+1} y(\lambda, m)$$
$$y(\lambda, m-1) = {}^{+}H^{m+1} y(\lambda, m)$$

Hence, the ladder of eigenfunctions

$$y(\lambda, m) \Longrightarrow y_l^m$$



move up and down.

Theorem 2

${}^{-}H^{m}$ and ${}^{+}H^{m}$ are adjoints.

$$\int_a^b \phi(x)\big({}^{-}Hf(x)\big)dx = \int_a^b \big({}^{-}H\phi(x)\big)f(x)dx$$

for all admissible ϕ and f,

$$\phi(a)f(a) = \phi(b)f(b) = 0$$

Theorem 3

$L(m) \uparrow$ implies y remains in L^2 and vanishes at a, b going up.

$L(m) \downarrow$ implies y remains in L^2 and vanishes at a, b going down.

Class I, $L(m) \uparrow$
$m = 1 : m$

Class II, $L(m) \downarrow$
$m = 1 : m$

Theorem 4

Class I . If $\lambda \leq \max\{L(m), L(m+1)\}$ and $y_l^m \in L^2$ then $\lambda_l = L(l+1)$.

Class II . If $\lambda \leq L(0)$ and $y_l^m \in L^2$ then $\lambda_l = L(l)$.

In both cases $y_l^l(x)$ can be found by quadrature.

Class I.

$$y_l^l(x) = C\exp\left(\int_a^x k(s, l+1)ds\right)$$

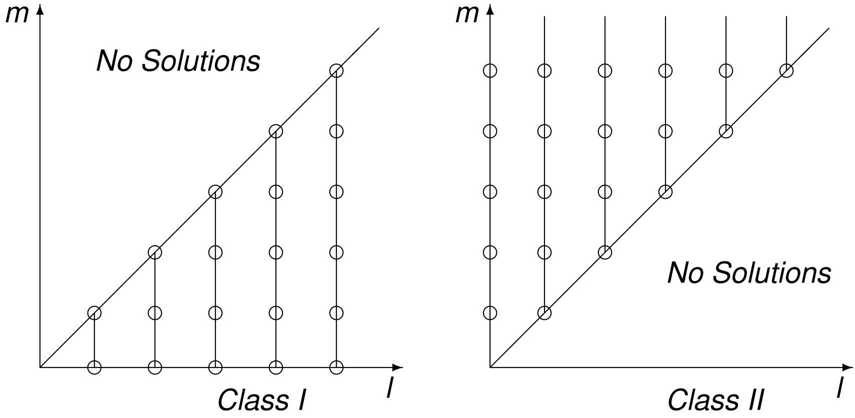
$$y_l^{m-1} = {}^{+}H^m y_l^m, \quad m \downarrow$$

Class II.

$$y_l^l(x) = C\exp\left(-\int_a^x k(s, l)ds\right)$$

$$y_l^{m+1} = {}^{-}H^{m+1} y_l^m, \quad m \uparrow$$

Theorem 4 (continued)



Matrix Interpretation

Uniform discretization

$$f(x) \sim \big(f(x_1), f(x_2), \ldots, f(x_n)\big)^T = f$$

$$k(x,m) \sim k_m = \big(k(x_1,m), k(x_2,m), \ldots, k(x_n,m)\big)^T$$

Backward Differences: $f'(x_j) \sim \dfrac{f(x_j) - f(x_{j-1})}{\delta x}$

$$({}^-\Delta f)(x_j) = \frac{f(x_j) - f(x_{j-1})}{\delta x}$$

${}^-\Delta$ is lower diagonal, $(\ldots, -1, 1, \ldots)/\delta x$

$${}^+H^m = \mathrm{diag}(k_m) + {}^-\Delta$$

Matrix Interpretation (continued)

By Theorem 2,

$$^{-}H^{m} = \left(^{+}H^{m} \right)^{T}$$

$$\left(^{+}H^{m+1} \right)\left(^{-}H^{m+1} \right) = \left(^{-}H^{m} \right)\left(^{+}H^{m} \right) - \left[L(m+1) - L(m) \right] I$$

$$\begin{bmatrix} \times & & & & \\ \times & \times & & & \\ & \times & \times & & \\ & & \times & \times & \\ & & & \times & \times \end{bmatrix} \begin{bmatrix} \times & \times & & & \\ & \times & \times & & \\ & & \times & \times & \\ & & & \times & \times \\ & & & & \times \end{bmatrix} = \begin{bmatrix} \times & \times & & & \\ & \times & \times & & \\ & & \times & \times & \\ & & & \times & \times \\ & & & & \times \end{bmatrix} \begin{bmatrix} \times & & & & \\ \times & \times & & & \\ & \times & \times & & \\ & & \times & \times & \\ & & & \times & \times \end{bmatrix} - \sigma_m I$$

LR with shifts, tridiagonal case.

Positive Def. $\sim$ Choleski LR