

Root finding via Product-Difference algorithm

- QMOM and DQMOM both rely on Gaussian quadrature to provide closure condition. An integral approximated by N-point quadrature is of the form, for $k \geq 1$:

$$k \int L^{k-1} \mathbf{f}(\mathbf{L}) \mathbf{n}(\mathbf{L}) d\mathbf{L} = k \sum_{i=1}^N L_i^{k-1} \mathbf{f}(\mathbf{L}) w_i$$

- The foundation of quadrature-based closure is that the abscissas L_i and weights w_i can be completely described in terms of the lower-order moments of the unknown distribution function $n(L)$. The moment of the distribution is written:

$$\mu_k = \int L^k \mathbf{n}(\mathbf{L}) d\mathbf{L} = \int L^{k-1} \cdot \mathbf{L} \cdot \mathbf{n}(\mathbf{L}) d\mathbf{L} = \sum_{i=1}^N L_i^{k-1} \mathbf{L} w_i = \sum_{i=1}^N L_i^k w_i$$

- The first $2N$ moments (μ_k with $k = 0$ through $k = 2N - 1$) determined N weight and N abscissas. A naïve approach is to try to solve the non-linear equations, which is not recommended. A much better approach is to deploy an “Product-difference” algorithm which will be showed on the next paragraph.
- The birth of “Product-difference” algorithm has nothing to do with solving population balance model. The goal is to calculate the *integral of an unknown function based on known moments*. Gordon¹ begins the derivation of the PD algorithm by considering the Stieltjes² integral.

$$I(z) = \int_0^\infty \frac{d\psi(E)}{z + E}$$

- The integral $I(z)$ is determined based on the moment of function $\psi(E)$ (non-decreasing) which is defined as a nondecreasing distribution within the interval of integration. z is a variable that can be represented by any number, real or imaginary, but it's constant with respect to integration.

$$\mu_k = \int_0^\infty E^k d\psi(E)$$

[1] Roy G. Gordon Error Bounds in Equilibrium Statistical Mechanics

[2] T. J. Stieltjes, Recherches sur les fractions continues, Annales de la Faculte des Sciences de Toulouse

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- By expanding the integrand in $I(z)$ based on finite geometric series, we receive the new integral approximation is a power series with only contain moment

$$I(z) \approx \frac{\mu_0}{z} - \frac{\mu_1}{z^2} + \frac{\mu_2}{z^3} - \frac{\mu_3}{z^4} + \dots + (-1)^N \frac{\mu_N}{z^{N+1}}$$

- As state by Scott and Wall¹, An arbitrary power series $P(x) = \sum_{n=0}^{\infty} c_n x^n$ has a unique corresponding continued fraction of the form:

$$K(x) = c_0 + \frac{a_1 x^{\alpha_1}}{1 + \frac{a_2 x^{\alpha_2}}{1 + \frac{a_3 x^{\alpha_3}}{\dots}}}$$

- Similarly, integration $I(z)$ has a corresponding continued fraction $C(z)$ since series convergence cannot be achieved in the summated form:

$$C(z) = \frac{\alpha_1}{z + \frac{\alpha_2}{1 + \frac{\alpha_3}{z + \frac{\alpha_4}{\dots}}}}$$

- The constant α_n is defined based on the moment μ_k . Product-difference (PD) algorithm is invented for conveniently evaluating α_n term. An infinite continued fraction $C(z)$ has a mathematical meaning only as a limit.

$$C(z) = \lim_{n \rightarrow \infty} C_n(z)$$

- In actual applications, one has available only a finite number of moments, truncated fraction obtained by setting $\alpha_{n+1} = 0, \alpha_{n+2} = 0$. To proceed further, it is preferable to separate the z constant from the continuing fraction in order to isolate the component dependent on the moments. The approximant $C(z)$ is represented as its even contraction $A^e(z)$.

$$A_n(z) = C_{2n}(z)$$

Root finding via Product-Difference algorithm

$$A_{2n}(z) = \frac{\alpha_1}{z + \alpha_2 - \frac{\alpha_2 \alpha_3}{z + \alpha_3 + \alpha_4 - \frac{\alpha_4 \alpha_5}{z + \alpha_5 + \alpha_6 - \dots}}}$$

- Multiplying the entire denominator of the right-hand side to the left, allows for the continued fraction to be represented as a composition of two matrices.

$$\left(z + \alpha_2 - \frac{\alpha_2 \alpha_3}{z + \alpha_3 + \alpha_4 - \frac{\alpha_4 \alpha_5}{z + \alpha_5 + \alpha_6 - \dots}} \right) A_{2n}(z) = \alpha_1$$

- $A^e(z)$ is the first component of vector \mathbf{x} which is the solution to the following set of n simultaneous linear equations. The proof of this equation can be found in Gordon's work¹ which is related to Gaussian elimination.

$$(z\mathbf{I} + \mathbf{M}) \cdot \mathbf{x} = \mathbf{e}_1 \alpha_1$$

- \mathbf{I} is $n \times n$ unit matrix and \mathbf{e}_1 is a unit vector with n rows, \mathbf{M} is $n \times n$ symmetric tridiagonal matrix.

$$M \equiv \begin{pmatrix} \alpha_2 & -(\alpha_2 \alpha_3)^{1/2} & 0 & 0 & 0 & \dots \\ -(\alpha_2 \alpha_3)^{1/2} & \alpha_3 + \alpha_4 & -(\alpha_4 \alpha_5)^{1/2} & 0 & 0 & \dots \\ 0 & -(\alpha_4 \alpha_5)^{1/2} & \alpha_5 + \alpha_6 & -(\alpha_6 \alpha_7)^{1/2} & 0 & \dots \\ \dots & \dots & \dots & \dots & \ddots & \dots \\ \dots & \dots & \dots & \dots & -(\alpha_{2n-2} \alpha_{2n-1})^{1/2} & \alpha_{2n-1} + \alpha_{2n} \end{pmatrix}$$

- The formal solution to these linear equations is:

$$\mathbf{x} = \alpha_1 (z\mathbf{I} + \mathbf{M})^{-1} \mathbf{e}_1$$

Root finding via Product-Difference algorithm

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$$\mathbf{x} = \alpha_1 (z\mathbf{I} + \mathbf{M})^{-1} \mathbf{e}_1$$

- Perform eigendecomposition on matrix \mathbf{M} , we have the formular below. In which, \mathbf{U} is square $n \times n$ matrix whose i^{th} column is the eigenvector \mathbf{q}_i of \mathbf{M} , $\mathbf{\Lambda}$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues, $\Lambda_{ii} = \lambda_i$

$$\mathbf{M} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1} \Rightarrow \mathbf{\Lambda} = \mathbf{U}^{-1}\mathbf{M}\mathbf{U}$$

- The linear equation becomes:

$$\mathbf{x} = \alpha_1 \mathbf{U}\mathbf{U}^{-1}(z\mathbf{I} + \mathbf{M})^{-1}\mathbf{U}\mathbf{U}^{-1}\mathbf{e}_1$$

$$x_1 = \sum_j \alpha_1 (z + \lambda_j)^{-1} u_{1j}^2$$

(*)

- In which, u_{1j} is the 1^{st} element of the vector column j^{th} of matrix \mathbf{U}

$$u_{1j} = (\mathbf{U})_{1j}$$

$$A_n(z) = x_1 = \alpha_1 \sum_{j=1}^n \frac{u_{1j}^2}{(z + \lambda_j)} = \sum_{j=1}^n \frac{w_i}{(z + \lambda_j)}$$

- We obtained the relation:

$$A_n(z) = I(z) = \int_0^\infty \frac{d\psi(E)}{z + E} = \sum_{j=1}^n \frac{w_i}{(z + \lambda_j)}$$

- The transformation step (*) is tricky, so details will be presented on the next slide.

Transformation step (*)

$$\mathbf{x} = \alpha_1 \mathbf{U} \mathbf{U}^{-1} (z\mathbf{I} + \mathbf{M})^{-1} \mathbf{U} \mathbf{U}^{-1} \mathbf{e}_1$$

- Set matrix $\mathbf{Q} = (z\mathbf{I} + \mathbf{M})$, we obtained:

$$\mathbf{x} = \alpha_1 \mathbf{U} \mathbf{U}^{-1} \mathbf{Q}^{-1} \mathbf{U} \mathbf{U}^{-1} \mathbf{e}_1$$

$$\mathbf{x} = \alpha_1 \mathbf{U} \mathbf{\Phi} \mathbf{U}^{-1} \mathbf{e}_1 (**)$$

- In which, $\mathbf{\Phi}$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues of matrix \mathbf{Q}^{-1} . Furthermore, the eigenvalues of the inverse matrix are equal to the inverse of the eigenvalues of the original matrix (easy to proof). Set φ_i is eigenvalues i^{th} of matrix \mathbf{Q} , eigenvalues of matrix \mathbf{Q}^{-1} a.k.a $(z\mathbf{I} + \mathbf{M})$ is φ_i^{-1} .
- Thanks for this Wikipedia pages [[Commuting matrices – Wikipedia](#)], we have two important pieces of the puzzle:
 - If \mathbf{A} and \mathbf{B} commute, they have a common eigenvector. If \mathbf{A} has distinct eigenvalues, and \mathbf{A} and \mathbf{B} **commute**, then \mathbf{A} 's eigenvectors are \mathbf{B} 's eigenvectors. \Rightarrow eigenvalue of $\mathbf{A} + \mathbf{B} =$ eigenvalue of $\mathbf{A} +$ eigenvalue of \mathbf{B}
 - The identity matrix commutes with all matrices. $\Rightarrow z\mathbf{I}$ **commutes** with \mathbf{M}
 - **Therefore** eigenvalue of $\mathbf{Q} =$ eigenvalue of $z\mathbf{I} +$ eigenvalue of \mathbf{M}
- Let's demonstrate them !!!
- For the sake of simplicity, matrix \mathbf{M} is 3×3 tridiagonal matrix with the form below:

$$\mathbf{M} \equiv \begin{bmatrix} a_1 & b_1 & \\ b_1 & a_2 & b_2 \\ & b_2 & a_3 \end{bmatrix}$$

- Perform eigendecomposition on matrix \mathbf{M}

$$\mathbf{M} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{-1} \equiv \begin{bmatrix} a_1 & b_1 & \\ b_1 & a_2 & b_2 \\ & b_2 & a_3 \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix}^{-1}$$

Transformation step (*)

- Because \mathbf{M} is asymmetry, \mathbf{U} is guaranteed to be an orthogonal matrix, therefore $\mathbf{U}^{-1} = \mathbf{U}^T$

$$\mathbf{M} = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{bmatrix} \begin{bmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{bmatrix}$$

- Perform eigendecomposition on matrix $z\mathbf{I}$, since it commute with \mathbf{M} , it should have the same \mathbf{U}

$$z\mathbf{I} \equiv z \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} = z\mathbf{U}\mathbf{I}\mathbf{U}^{-1} = z \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{bmatrix}$$

- Perform eigendecomposition on matrix $\mathbf{Q} = z\mathbf{I} + \mathbf{M}$

$$\mathbf{Q} = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} z + \lambda_1 & & \\ & z + \lambda_2 & \\ & & z + \lambda_3 \end{bmatrix} \begin{bmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{bmatrix}$$

- Perform eigendecomposition on matrix $\mathbf{Q}^{-1} = (z\mathbf{I} + \mathbf{M})^{-1}$

$$\mathbf{Q}^{-1} = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} \frac{1}{z + \lambda_1} & & \\ & \frac{1}{z + \lambda_2} & \\ & & \frac{1}{z + \lambda_3} \end{bmatrix} \begin{bmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{bmatrix}$$

Transformation step (*)

- It's obvious that, eigenvector of matrix \mathbf{Q}^{-1} is:

$$\Phi = \begin{bmatrix} (z + \lambda_1)^{-1} & & \\ & (z + \lambda_3)^{-1} & \\ & & (z + \lambda_3)^{-1} \end{bmatrix}$$

- Plug it back to the equation (**) $\mathbf{x} = \alpha_1 \mathbf{U} \Phi \mathbf{U}^{-1} \mathbf{e}_1$, the equation is written in full matrix form.

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \alpha_1 \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} (z + \lambda_1)^{-1} & & \\ & (z + \lambda_3)^{-1} & \\ & & (z + \lambda_3)^{-1} \end{bmatrix} \begin{bmatrix} u_{11} & u_{21} & u_{31} \\ u_{12} & u_{22} & u_{32} \\ u_{13} & u_{23} & u_{33} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \alpha_1 \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} (z + \lambda_1)^{-1} & & \\ & (z + \lambda_3)^{-1} & \\ & & (z + \lambda_3)^{-1} \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{12} \\ u_{13} \end{bmatrix}$$

1st eigenvector

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \alpha_1 \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{bmatrix} \begin{bmatrix} u_{11}(z + \lambda_1)^{-1} \\ u_{12}(z + \lambda_3)^{-1} \\ u_{13}(z + \lambda_3)^{-1} \end{bmatrix}$$

- We are only interesting in x_1 , only the first row of the matrix \mathbf{U} is performed the matrix multiplication.

$$x_1 = u_{11}^2(z + \lambda_1)^{-1} + u_{12}^2(z + \lambda_1)^{-1} + u_{13}^2(z + \lambda_1)^{-1}$$

- Let's generalize:

$$x_1 = \sum_j \alpha_1 (z + \lambda_j)^{-1} u_{1j}^2$$

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- Follow the slide that was mentioned before, we already obtained:

$$A_n(z) = I(z) = \int_0^\infty \frac{d\psi(E)}{z + E} = \sum_{j=1}^n \frac{w_j}{(z + \lambda_j)}$$

- Then we can obtain the generalization in which $(z + E)^{-1}$ is $f(E)$

$$\int_0^\infty f(E) d\psi(E) = \sum_{j=1}^n f(\lambda_j) w_j$$

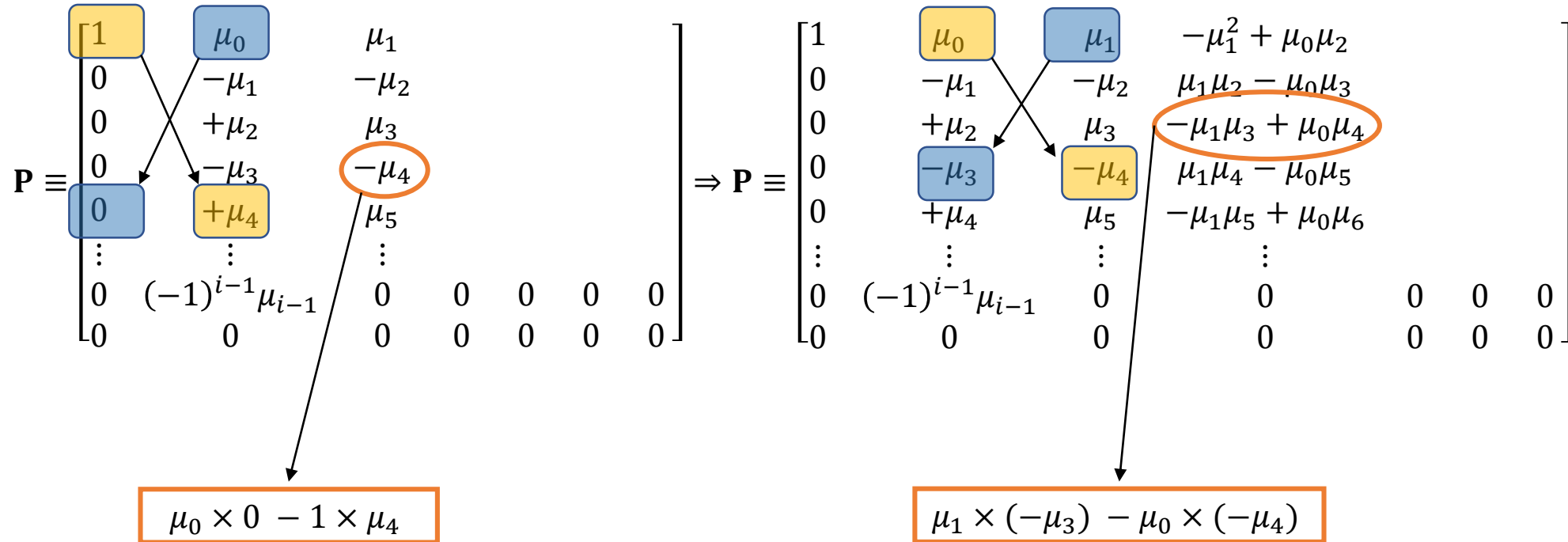
- Let's go back to the moment equation

$$\mu_k = \int_0^\infty E^k d\psi(E) = \sum_{j=1}^n \lambda_j^k w_j$$

- The expression above magically becomes a powerful tool to overcome the closure problem of MOM. In the expression, abscissa λ_j is the eigenvalue j^{th} of matrix \mathbf{M} , which is constructed based on α_n , and α_n is determined in term of μ_k . Weight w_j is the product between $\alpha_1 = \mu_0$ and the square of the first component of eigenvector j^{th} , $U_{1,j}^2$.
- The next slide is the detail procedure to construct the matrix \mathbf{M}

Product-Difference algorithm

- Problem: Find determined N weight and N abscissas of N-point Gaussian quadrature. We need $2N$ moments from μ_0 to μ_{2N-1}
- **Part A:** Construct a square matrix \mathbf{P} with size $2N+1$
 - The first column is 0, except $\mathbf{P}(1,1)$
 - The second column contains the moments with alternating sign: $\mathbf{P}(i, 2) = (-1)^{i-1} \mu_{i-1}$
 - The element from the column 3 is determined based on the product-difference recursion relation:
$$\mathbf{P}(i, j) = \mathbf{P}(1, j-1) \mathbf{P}(i+1, j-2) - \mathbf{P}(1, j-2) \mathbf{P}(i+1, j-1)$$
 - The values of the elements in the N^{th} column are calculated based on the elements in the $N-1$ and $N-2$ columns



Product-Difference algorithm

- Problem: Find determined N weight and N abscissas of N -point Gaussian quadrature. We need $2N$ moments from μ_0 to μ_{2N-1}
- **Part B:** Construct a tridiagonal matrix \mathbf{M} with size $N \times N$
 - Calculate the coefficient α_n based on \mathbf{P} (α_n is the coefficient from continues fraction $A_n(z)$)

$$\alpha_1 = 0 \text{ (follow the work from Marchisio¹)}$$

$$\alpha_i = \frac{P(1, i+1)}{P(1, i)P(1, i-1)}, \quad i \in 2, \dots, 2N$$

- There are $2N$ coefficient α_n are obtained from $2N+1$ elements of the first row of matrix \mathbf{P} .
- The Jacobian \mathbf{M} was then constructed with the form:

$$\mathbf{M} = \begin{pmatrix} a_1 & b_1 & 0 & 0 \\ b_1 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & b_{i-1} \\ 0 & 0 & b_{i-1} & a_i \end{pmatrix}$$

- In which:

$$a_i = \alpha_{2i} + \alpha_{2i-1}, \quad i \in 1, \dots, 2N-1$$

$$b_i = -\sqrt{\alpha_{2i+1}\alpha_{2i-1}}, \quad i \in 1, \dots, 2N-2$$

- In **MATLAB**: $[\mathbf{\Lambda}, \mathbf{Q}] = \text{eig}(\mathbf{M})$, diagonal matrix $\mathbf{\Lambda}$ of eigenvalues and matrix \mathbf{Q} whose columns are the corresponding right eigenvectors
 - Abscissa $\lambda_i = \mathbf{\Lambda}(i, i)$
 - Weight $w_i = \mu_0 \mathbf{Q}(1, i)$
 - $\mu_0 = 1$ (assuming $n(L)$ is a normalize distribution)