# CS 3331 Numerical Methods

# Lecture 8: Approximation

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# Outline

- Linear least square approximation
- Functional approximation
  - Function norm and orthogonal polynomial
  - Legendre polynomial
  - Chebyshev polynomial
- Rational function approximation

# Linear Least Square Problems

# Goal

- Given a set of observed data $(x_1, y_1), (x_2, y_2), \cdots (x_m, y_m)$, the linear least square problem is to find the coefficient $a_1, a_2, \cdots, a_n$ such that the linear combination of a set of basis functions, $\{\phi_1, \phi_2, \cdots, \phi_n\}$,

$$u(x) = \sum_{i=1}^{n} a_i \phi_i(x),$$

gives the best model to the data.

- *Best* is measured by the least square errors

$$\min_{a_1, a_2, \cdots, a_n} \sum_{j=1}^{m} |y_j - u(x_j)|^2$$

# Approximation by a straight line LVF pp.350-355

- The straight line model is $a_1 x + a_2$ ($\phi_1 = x$ and $\phi_2 = 1$).
- Find $a_1, a_2$ to minimize the function

$$f(a_1, a_2) = \sum_{j=1}^{m} [(a_1 x_j + a_2) - y_j]^2$$

- The minimum is at the solution of the system

$$\begin{cases} \dfrac{\partial f}{\partial a_1} = 2 \displaystyle\sum_{j=1}^{m} [(a_1 x_j + a_2) - y_j] x_j = 0 \\ \dfrac{\partial f}{\partial a_2} = 2 \displaystyle\sum_{j=1}^{m} [(a_1 x_j + a_2) - y_j] = 0 \end{cases}$$

# Normal equation

- Define $\mathbf{A} = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_m & 1 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$. The equations can be written as a linear system $\mathbf{A}^T\mathbf{A}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \mathbf{A}^T\mathbf{b}$

$$\mathbf{A}^T\mathbf{A} = \begin{pmatrix} \sum_{j=1}^{m} x_j^2 & \sum_{j=1}^{m} x_j \\ \sum_{j=1}^{m} x_j & m \end{pmatrix} \text{ and } \mathbf{A}^T\mathbf{b} = \begin{pmatrix} \sum_{j=1}^{m} x_j y_j \\ \sum_{j=1}^{m} y_j \end{pmatrix}$$

- $\mathbf{A}^T\mathbf{A}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \mathbf{A}^T\mathbf{b}$ is called the *normal equation*.

# Approximation by a parabola LVF pp.356-359

- The model is $a_1x^2 + a_2x + a_3$ ($\phi_1 = x^2$, $\phi_2 = x$, $\phi_3 = 1$).
- Find $a_1, a_2, a_3$ to minimize the function

$$f(a_1, a_2, a_3) = \sum_{j=1}^{m} [(a_1x_j^2 + a_2x_j + a_3) - y_j]^2$$

- The minimizer is the solution of $\begin{cases} \partial f/\partial a_1 = 0 \\ \partial f/\partial a_2 = 0 \\ \partial f/\partial a_3 = 0 \end{cases}$

- Normal equation $\mathbf{A}^T\mathbf{A}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \mathbf{A}^T\mathbf{b}$, where $\mathbf{A} = \begin{pmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \\ x_m^2 & x_m & 1 \end{pmatrix}$.

# General form

- Approximate $(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)$ by a model $a_1\phi_1(x) + a_2\phi_2(x) + \ldots + a_n\phi_n(x)$

- $\mathbf{A} = \begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_n(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_n(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(x_m) & \phi_2(x_m) & \cdots & \phi_n(x_m) \end{pmatrix}, \mathbf{x} = \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_n \end{pmatrix}, \mathbf{b} = \begin{pmatrix} y_1 \\ y_2 \\ \cdots \\ y_m \end{pmatrix}$

- The least square problem $\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|^2$ can be solved by the normal equation $\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$.

- Let $\mathbf{y} = \mathbf{b} - \mathbf{A}\mathbf{x}$. The minimization of $\mathbf{y}^T\mathbf{y}$ is at $\frac{\partial(\mathbf{y}^T\mathbf{y})}{\partial \mathbf{x}} = 0$.

$$\mathbf{y}^T\mathbf{y} = (\mathbf{b} - \mathbf{A}\mathbf{x})^T(\mathbf{b} - \mathbf{A}\mathbf{x}) = \mathbf{b}^T\mathbf{b} - 2\mathbf{x}^T\mathbf{A}^T\mathbf{b} + \mathbf{x}^T\mathbf{A}^T\mathbf{A}\mathbf{x}$$

$$\frac{\partial \mathbf{y}^T\mathbf{y}}{\partial \mathbf{x}} = -2\mathbf{A}^T\mathbf{b} + 2\mathbf{A}^T\mathbf{A}\mathbf{x} = 0$$

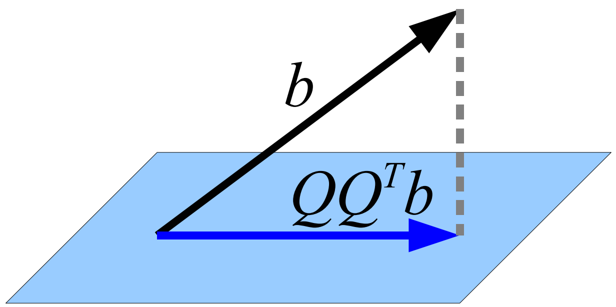
  The minimizer of $\|\mathbf{b} - \mathbf{A}\mathbf{x}\|^2$ is the solution of $\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$

- $\mathbf{A} = \mathbf{Q}\mathbf{R}$ where $\mathbf{Q}$ is an $m \times n$ matrix with orthonormal columns, $\mathbf{R}$ is an $n \times n$ upper triangular matrix.
  - Normal equation becomes $\mathbf{R}^T\mathbf{Q}^T\mathbf{Q}\mathbf{R}\mathbf{x} = \mathbf{R}^T\mathbf{Q}^T\mathbf{b}$.
  - $\mathbf{R}^T$ is invertible and $\mathbf{Q}^T\mathbf{Q} = I \Rightarrow$ Solving $\mathbf{R}\mathbf{x} = \mathbf{Q}^T\mathbf{b}$.
  - More stable/cheaper than using normal equation.

# Geometric interpretation

- Note the minimizer is not at the solution of $\mathbf{Ax} = \mathbf{b}$, but $\mathbf{Ax} = \mathbf{QQ}^T\mathbf{b}$.
  - From $\mathbf{Rx} = \mathbf{Q}^T\mathbf{b}$, pre-multiplying $\mathbf{Q}$ to both sides.
- $\mathbf{QQ}^T$ is an orthogonal projection matrix.

  - Projects $\mathbf{b}$ to $\mathcal{S} = \text{span}(\phi_1, \phi_2, \ldots, \phi_n)$
  - The error vector $\mathbf{b} - \mathbf{Ax}$ is orthogonal to $\mathcal{S}$ when $\|\mathbf{b} - \mathbf{Ax}\|$ is minimized.
  - The minimum error is $\|\mathbf{b} - \mathbf{QQ}^T\mathbf{b}\|$



# Total least square problems

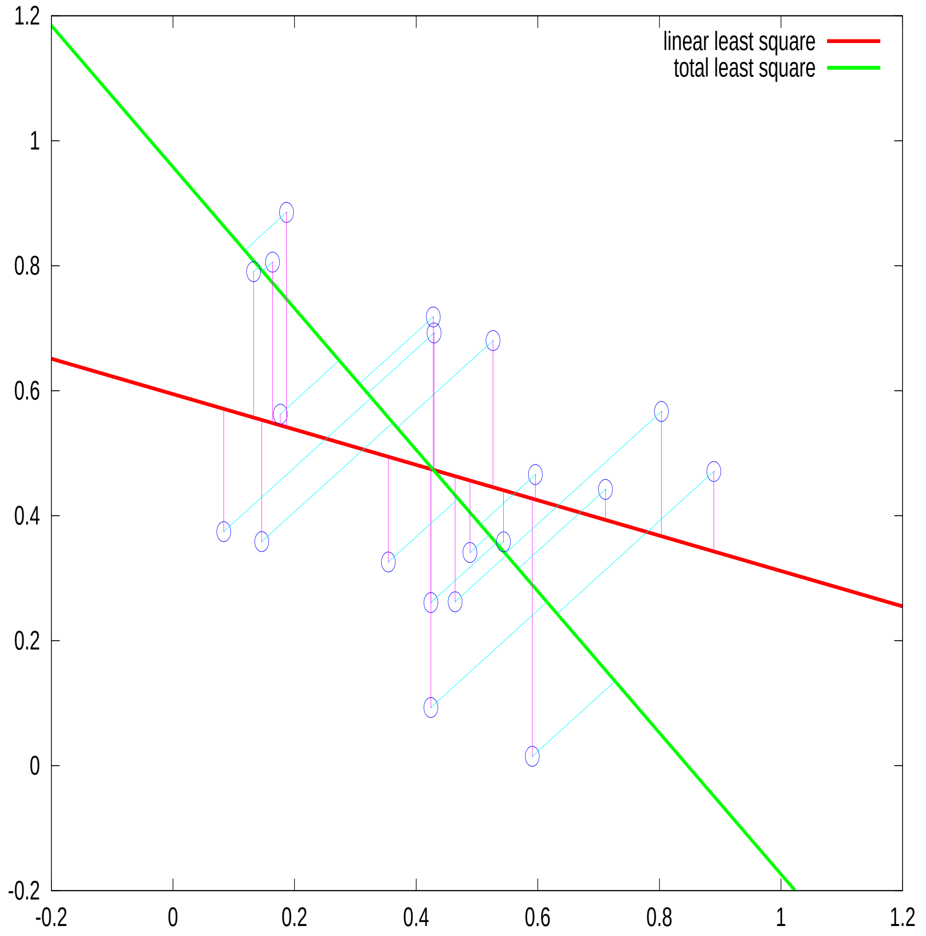
- $\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}, \bar{y} = \frac{\sum_{i=1}^{n} y_i}{n}$.

$$\mathbf{A} = \begin{pmatrix} x_1 - \bar{x} & y_1 - \bar{y} \\ x_2 - \bar{x} & y_2 - \bar{y} \\ \vdots & \vdots \\ x_n - \bar{x} & y_n - \bar{y} \end{pmatrix}$$

- Covariance matrix

$$\mathbf{C} = \mathbf{A}^T \mathbf{A}$$

- The eigenvector of $\mathbf{C}$, corresponding to the largest eigenvalue, is the slope of the line. $\Rightarrow$ The first singular vector of $\mathbf{A}$.



# Functional Approximation

# Basic idea

- Want to approximate a continuous real function $f(x)$ by a set of continuous functions $P_1(x), P_2(x), \ldots, P_n(x)$.
- Mathematically, find real numbers $a_1, a_2, \ldots, a_n$ such that

$$\min_{a_1, a_2, \ldots, a_n \in \mathbb{R}} \| f(x) - (a_1 P_1(x) + a_2 P_2(x) + \cdots + a_n P_n(x)) \|$$

- Use the same idea from points set

1. Find an orthogonal basis of $P_1(x), P_2(x), \ldots, P_n(x)$.
2. Let $g(x)$ be the $f(x)$ projected to the orthogonal basis.
3. Solve $g(x) = a_1 P_1(x) + a_2 P_2(x) + \cdots + a_n P_n(x)$.

# Function norm and inner product

- How to measure the "size" of a continuous $f(x)$ on $[a, b]$?
  - 1-norm: $\|f(x)\|_1 = \int_a^b |f(x)| dx$
  - 2-norm: $\|f(x)\|_2 = (\int_a^b f^2(x) dx)^{1/2}$
  - $\infty$-norm: $\|f(x)\|_\infty = \sup_{x \in [a,b]} |f(x)|$
- Suppose $f(x)$, $g(x)$, $w(x)$ are defined on $[a, b]$, $w(x) > 0$.
  - Inner product: $\langle f(x), g(x) \rangle = \int_a^b f(x) g(x) dx$
  - Weighted inner product: $\langle f(x), g(x) \rangle_w = \int_a^b w(x) f(x) g(x) dx$.

# Orthogonal functions LVF pp.366

- Functions $f_1, f_2, \ldots, f_n$ are defined on $[a, b]$.
  - They are *linearly independent* if $\forall x \in [a, b]$
  $$c_1 f_1(x) + c_2 f_2(x) + \cdots + c_n f_n(x) = 0$$
  implies $c_1 = c_2 = \ldots = c_n = 0$.
- $f_1, f_2, \ldots, f_n$ are orthogonal if $\forall i, j$
  $$\langle f_i(x), f_j(x) \rangle = \int_a^b f_i(x) f_j(x) dx = \begin{cases} 0, & \text{if } i \neq j; \\ a_i \neq 0, & \text{if } i = j. \end{cases}$$
  - Orthogonal implies linearly independent.
  - If $a_i = 1$ for all $i$, they are orthonormal.

# Gram-Schmidt process LVF pp.366

- Same as what we have learned in chap 4, but with different definition of inner product and norm.
- Given a set of functions, $f_1, f_2, \ldots, f_n$, construct a set of orthonormal functions $g_1, g_2, \ldots, g_n$ that span the same "space".

1. $g_1 = f_1/\|f_1\|$
2. For $i = 2, \ldots, n$
   (a) $g_i = f_i - \sum_{k=1}^{i-1} \langle g_k, f_i \rangle g_k.$
   (b) $g_i = g_i/\|g_i\|$

# Orthogonal polynomial LVF pp.366

- $1, x, x^2, \ldots, x^n$ are linearly independent on $[-1, 1]$, but not orthogonal.
- Using Gram-Schmidt process, we have

$$
\begin{aligned}
f_0(x) &= 1/\sqrt{2} \\
f_1(x) &= \sqrt{3/2}x \\
f_2(x) &= \sqrt{\frac{45}{8}}\left(x^2 - \frac{1}{3}\right) \\
\vdots &= \vdots
\end{aligned}
$$

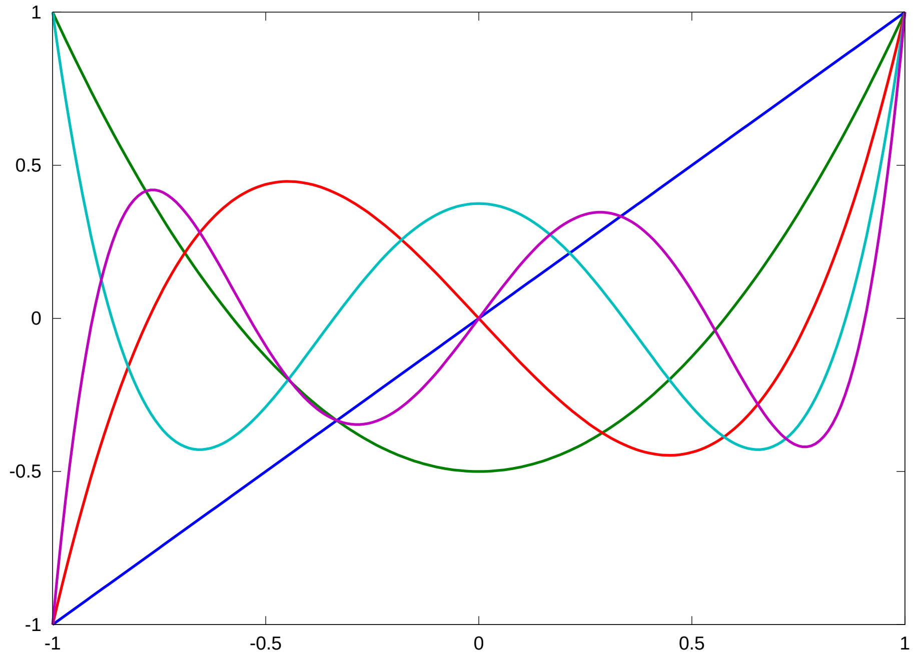
- Recurrence: $a_k f_{k+1} + (b_k - x) f_k + c_k f_{k-1} = 0$ for $k \geq 1$.
- The roots of $f_k$ and $f_{k-1}$ are interleaving.

# Legendre polynomials LVF pp.368

- $P_0(x) = 1$ and $P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}\left[(x^2-1)^n\right]$ for $n \geq 1$.
- $(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$

$$
\begin{aligned}
P_0 &= 1 \\
P_1 &= x \\
P_2 &= 1/2(3x^2-1) \\
P_3 &= 1/2(5x^3-3x) \\
P_4 &= 1/8(25x^4-30x^2-3) \\
P_5 &= 1/8(63x^5-70x^3-15x)
\end{aligned}
$$

$\langle P_i, P_i\rangle = \frac{2}{2i+1}$



# Approximation by Legendre polynomials LVF pp.369

- For a function $f(x)$ in $[-1, 1]$. Find $c_0, c_1, \ldots, c_n$ such that

$$\min_{c_0, c_1, \ldots, c_n} \|f(x) - (c_0 P_0(x) + c_1 P_1(x) + \cdots + c_n P_n(x))\|^2$$

- Let $e(x) = f(x) - (c_0 P_0(x) + c_1 P_1(x) + \cdots + c_n P_n(x))$.
  To minimize $\|e(x)\|$, $\langle e(x), P_i(x)\rangle$ must be 0.

$$\begin{aligned}
\langle e(x), P_i(x)\rangle &= \langle f(x) - (c_0 P_0(x) + c_1 P_1(x) + \cdots + c_n P_n(x)), P_i(x)\rangle \\
&= \langle f(x), P_i(x)\rangle - c_0\langle P_0(x), P_i(x)\rangle - \cdots - \langle P_n(x), P_i(x)\rangle \\
&= \langle f(x), P_i(x)\rangle - c_i\langle P_i(x), P_i(x)\rangle = 0
\end{aligned}$$

- The coefficient $c_i = \dfrac{\langle f(x), P_i(x)\rangle}{\langle P_i(x), P_i(x)\rangle} = \dfrac{2i+1}{2}\langle f(x), P_i(x)\rangle$.

# Chebyshev polynomials LVF pp.370

- Definition: $T_n(x) = \cos(n \arccos(x))$.
- Change variables: let $\theta = \arccos(x)$. $T_n(\theta) = \cos(n\theta)$.

$$\begin{aligned}
T_0(x) &= \cos(0) = 1 \\
T_1(x) &= \cos(\theta) = x \\
T_2(x) &= \cos(2\theta) = 2\cos^2(\theta) - 1 = 2x^2 - 1 \\
T_3(x) &= \cos(3\theta) = 4\cos^3(\theta) - 3\cos(\theta) = 4x^3 - 3x
\end{aligned}$$

- Recurrence: $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$
  - $\cos((n+1)\theta) + \cos((n-1)\theta) = 2\cos(\theta)\cos(n\theta)$.

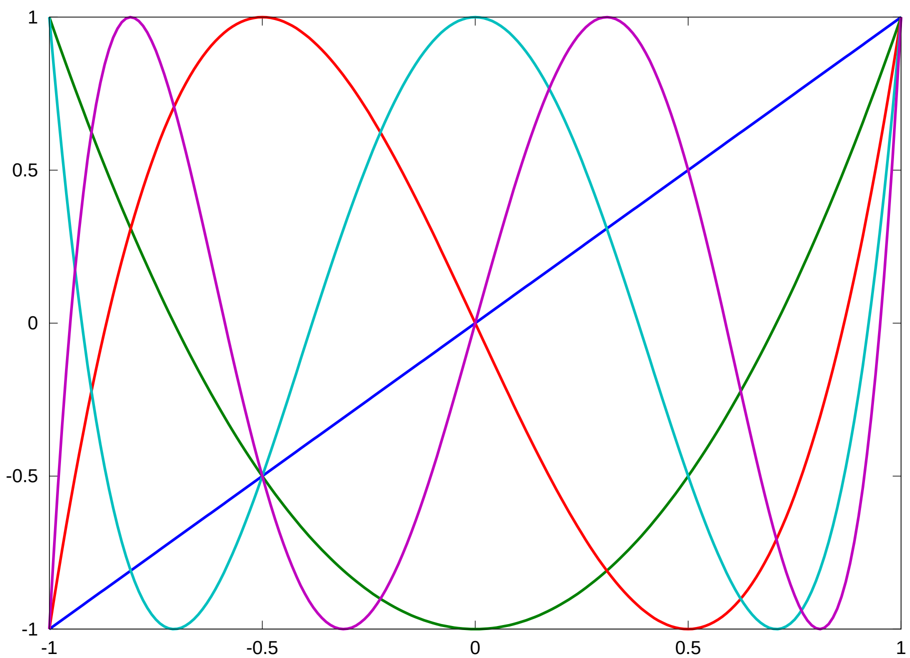
- Orthogonality $\int_{-1}^{1} \frac{T_m(x)T_n(x)}{\sqrt{1-x^2}}dx = \begin{cases} 0, & \text{if } m \neq n; \\ \pi/2, & \text{if } m = n \neq 0; \\ \pi, & \text{if } m = n = 0. \end{cases}$

- The roots of $T_n(x)$ are $\cos\left(\frac{2k-1}{2n}\pi\right)$, for $k = 1, \ldots, n$.

- The function,

$$f_n(x) = T_n(x)/2^{n-1},$$

has minimal $\infty$-norm, $2^{-(n-1)}$, on $[-1, 1]$ among all the polynomial of degree $n$ with leading coefficient 1.



# Rational Function Approximation

# Taylor approximation LVF pp.375

- The Taylor polynomial of degree $n$ that approximates $f(x)$ near $x = a$.

  $$t_n(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n$$

  - The error is bounded by $\dfrac{f^{(n+1)}(\eta)}{(n+1)!}(x-a)^{n+1}$ for some $\eta$ between $x$ and $a$.

- Not a good approximation if the function has singularities.

- Here we only consider $a = 0$ case (Maclaurin series).

# Pade approximation LVF pp.372

- Approximate $f(x)$ by a rational function.

$$r_{m,n}(x) = \frac{p_m(x)}{q_n(x)} = \frac{a_m x^m + \ldots + a_1 x + a_0}{b_n x^n + \ldots + b_1 x + 1}$$

- Let $k = m + n$ and $t(x)$ be the $k$th order Taylor polynomial of $p_m(x)/q_n(x)$, $t_k(x) = c_k x^k + \cdots + c_2 x^2 + c_1 x + c_0$.
  - We want $r_{m,n}(x)$ to have the same function value and derivatives of all orders up to $k$ as $t_k(x)$.

$$r_{m,n}(0) = t_k(0), r'_{m,n}(0) = t'_k(0), \cdots, r^{(k)}_{m,n}(0) = t^{(k)}_k(0).$$

  - $k + 1$ unknowns and $k + 1$ equations.

- To make things easier, use the expression $q_n(x)t_k(x) = p_m(x)$.

$$(b_n x^n + \ldots + b_1 x + 1)(c_k x^k + \cdots + c_1 x + c_0) = a_m x^m + \ldots + a_1 x + a_0$$

- Let $g(x) = q_n(x)t_k(x)$.

$$\begin{aligned} g'(x) &= q_n(x)t_k'(x) + q_n'(x)t_k(x) \\ g''(x) &= q_n(x)t_k''(x) + 2q_n'(x)t_k'(x) + q_n''(x)t_k(x) \\ &\vdots \\ g^{(n)}(x) &= \sum_{j=0}^{n} \frac{n!}{j!(n-j)!} q_n^{(j)}(x)t_k^{(n-j)}(x) \end{aligned}$$

- General relations: $a_j = c_j + \sum_{i=0}^{j-1} c_i b_{j-i}$, for $j = 0, 1, \ldots, k$.

# Rational function approximation

| $e^x$ at 0 | first order | second order | third order |
|---|---|---|---|
| Taylor approx | $1+x$ | $1+x+\frac{1}{2}x^2$ | $1+x+\frac{1}{2}x^2+\frac{1}{6}x^3$ |
| Inverse approx | $1/(1-x)$ | $1/(1-x+\frac{1}{2}x^2)$ | $1/(1-x+\frac{1}{2}x^2-\frac{1}{6}x^3)$ |
| Rational approx | $\frac{1+x/2}{1-x/2}$ | $\frac{1+x/2+x^2/12}{1-x/2+x^2/12}$ | $\frac{1+x/2+x^2/10+x^3/120}{1-x/2+x^2/12-x^3/120}$ |