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What degree to choose in polynomial calibration

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Outline

- Polynomial calibration
  - What does it involve?
  - Uncertainty structures
  - Parametrisation
- Polynomial degree not known in advance
  - Assessment of different degrees
- Conclusions
- References

Polynomial calibration
What does it involve?

- Can be thought of as a two-stage process
- Stage 1: Determination of polynomial calibration function
- Stage 2: Use of polynomial calibration function

Polynomial calibration
What does it involve?

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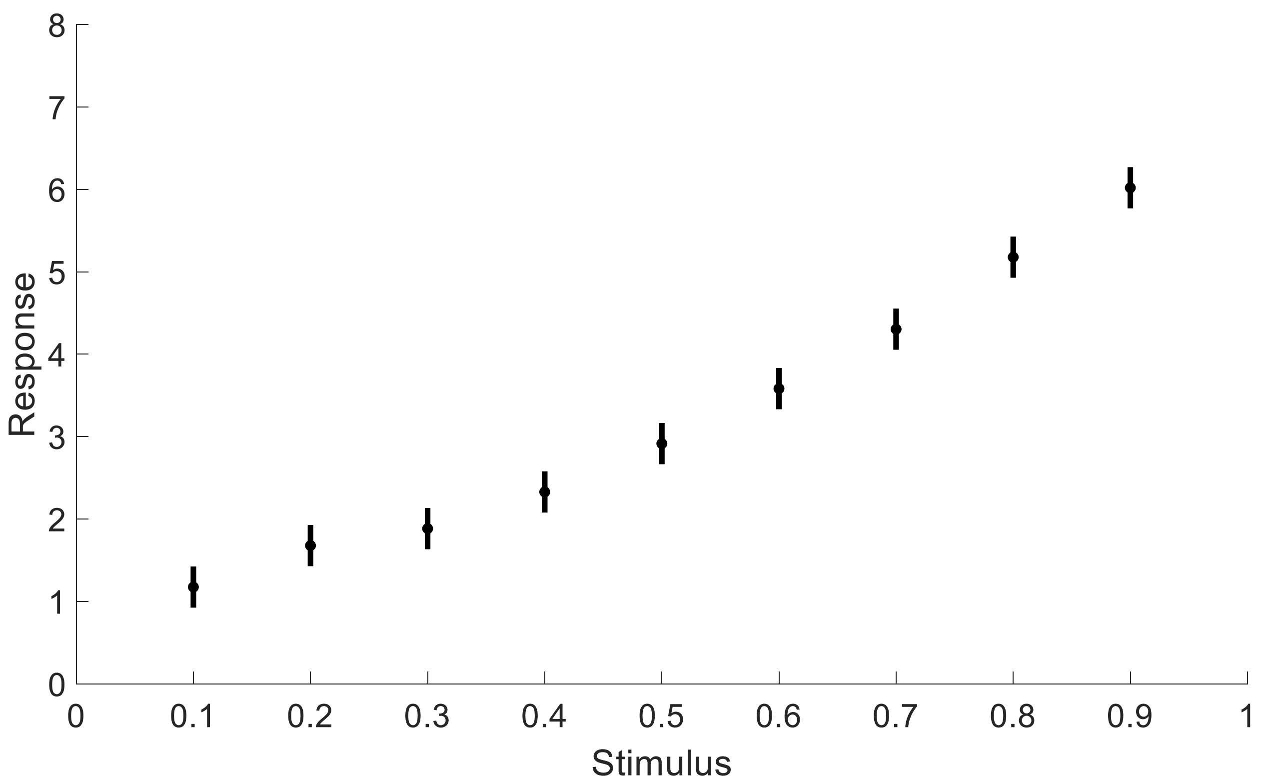
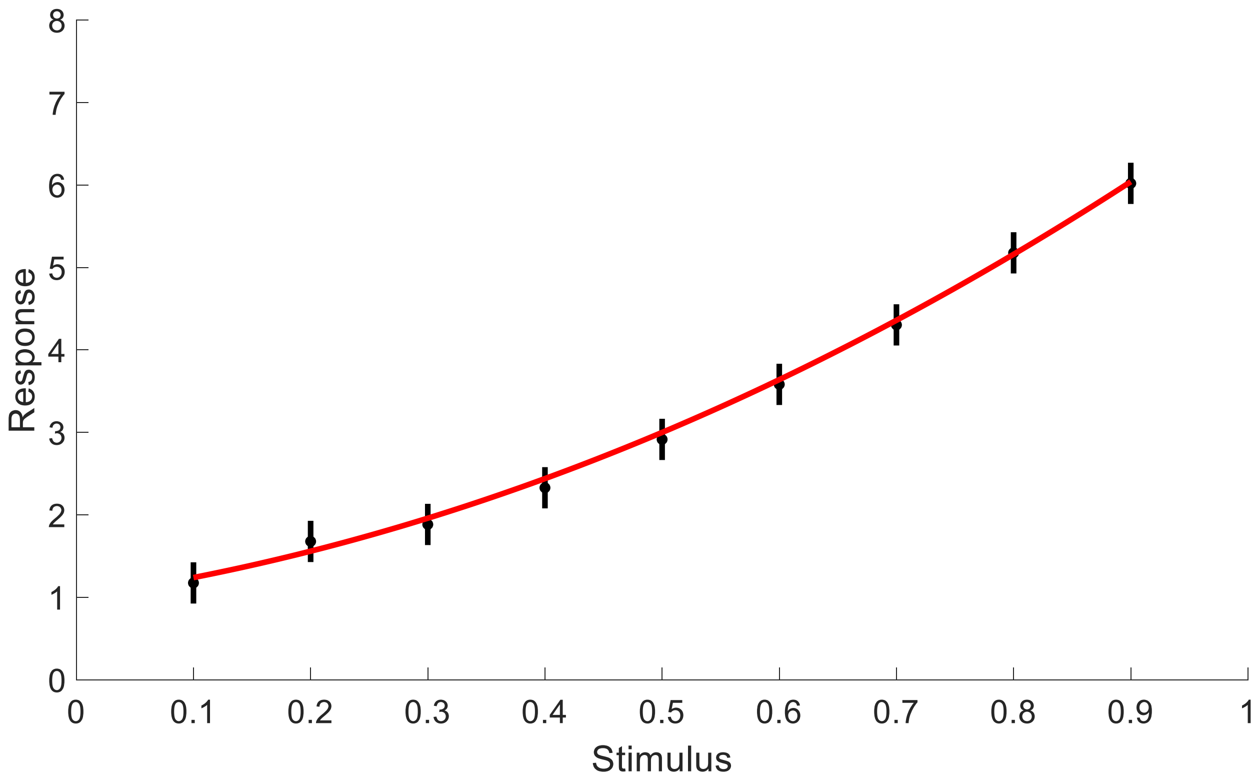
Measurement data
Stimulus and response values, with uncertainties associated with response values



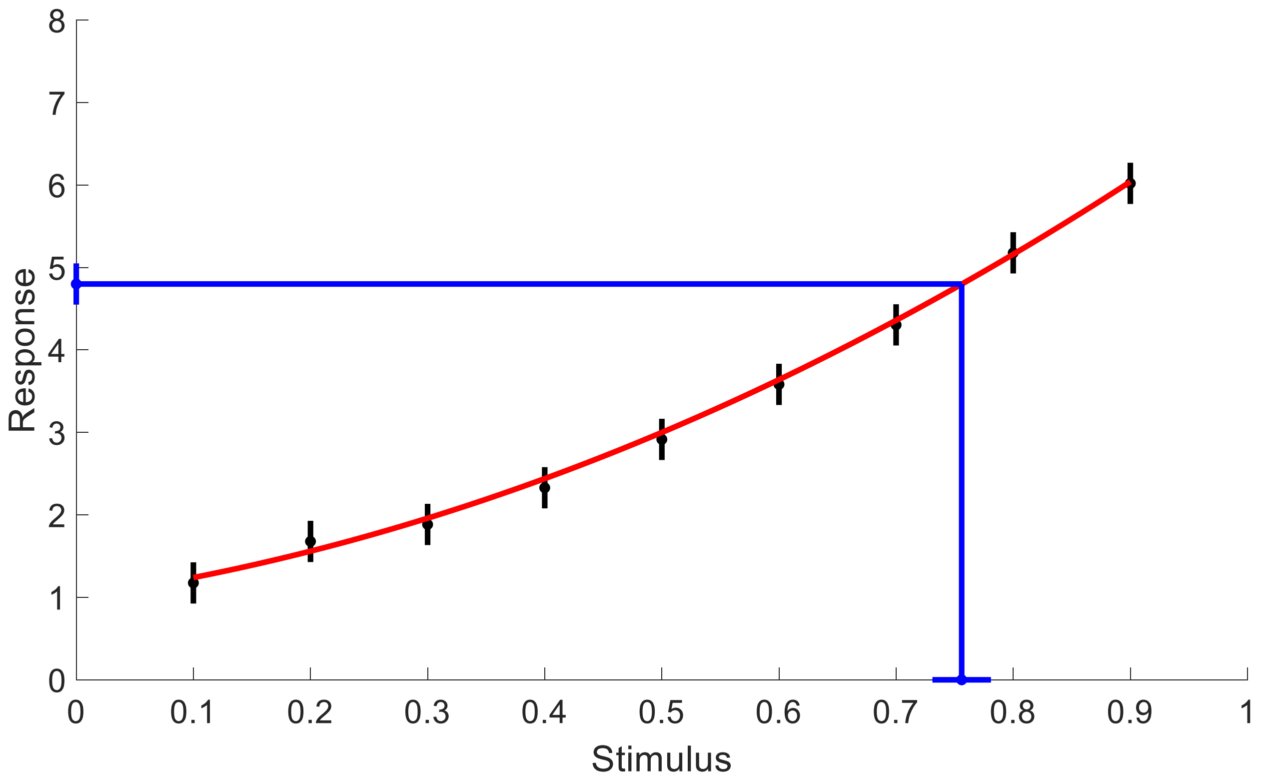
Polynomial calibration
What does it involve?

Polynomial calibration function (degree 2)
Estimates of coefficients and covariance matrix



Polynomial calibration
What does it involve?

Use of calibration function to determine value of stimulus (and associated uncertainty) corresponding to measured value of response (and associated uncertainty)



Polynomial calibration
What does it involve?

- Calibration function may be used in other ways
- Variations arise, e.g., where the calibration function is constrained to pass through the origin
- This presentation is restricted to unconstrained calibration functions

Polynomial calibration
Uncertainty structures

- Earlier example assumed that uncertainties associated with stimulus values are negligible
- Other uncertainty structures occur within metrology
- Can be “ranked” in increasing order of complexity

Polynomial calibration
Uncertainty structure 1

- Stimulus values $x_1, \ldots, x_m$

- Response values $y_1, \ldots, y_m$
- Standard uncertainties $u(y_1), \ldots, u(y_m)$

Covariance matrix $\boldsymbol{V}_{\boldsymbol{y}}$ is diagonal

Polynomial calibration
Uncertainty structure 2

- Stimulus values $x_1, \ldots, x_m$

- Response values $y_1, \ldots, y_m$
- Standard uncertainties $u(y_1), \ldots, u(y_m)$
- Covariances $u(y_i, y_j),\ i = 1, \ldots, m,\ j = 1, \ldots, m,\ i \neq j$

Covariance matrix $\boldsymbol{V}_y$ is not diagonal

Polynomial calibration
Uncertainty structure 3

- Stimulus values $x_1, \ldots, x_m$
- Standard uncertainties $u(x_1), \ldots, u(x_m)$

Covariance matrix $\boldsymbol{V}_x$ is diagonal

- Response values $y_1, \ldots, y_m$
- Standard uncertainties $u(y_1), \ldots, u(y_m)$

Covariance matrix $\boldsymbol{V}_y$ is diagonal

Polynomial calibration
Uncertainty structure 4

- Stimulus values $x_1, \ldots, x_m$
- Standard uncertainties $u(x_1), \ldots, u(x_m)$
- Covariances $u\left(x_i, x_j\right),\ i = 1, \ldots, m,\ j = 1, \ldots, m,\ i \neq j$

Covariance matrix $\boldsymbol{V}_x$ is not diagonal

- Response values $y_1, \ldots, y_m$
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Covariance matrix $\boldsymbol{V}_y$ is not diagonal

Polynomial calibration
Uncertainty structures

- Problems arising from the various uncertainty structures have been considered for many years by NMIs
  - Software made freely available

- Can be solved using linear algebra, either directly (uncertainty structures 1 and 2) or iteratively (3 and 4)

Polynomial calibration Parametrisation [1]

- Traditional representation

$$p(x, \mathbf{A}) = A_0 + A_1 x + \cdots + A_n x^n$$

- **But** for very large (or very small) values of $|x|$, x^r becomes very large (very small) as r increases
  - Potential numerical issues*

- **Also** not always straightforward to interpret coefficient values

- Look for alternative parametrisation

*depending on nature of data and/or polynomial degree

Polynomial calibration Parametrisation [2]

- Representation in terms of scaled stimulus values, i.e.,

$$p(x, \mathbf{B}) = B_0 + B_1 \hat{x} + \cdots + B_n (\hat{x})^n,$$

where

$$\hat{x} = \frac{x}{\max(|x_i|)}$$

- All $\hat{x}$-values, and therefore powers of $\hat{x}$-values, lie in the interval $[-1, 1]$

- Easier to understand contributions of each term

Polynomial calibration Parametrisation [3]

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- Representation in terms of normalised stimulus values, i.e.,

$$p(x, \mathbf{C}) = C_0 + C_1 t + \cdots + C_n t^n,$$

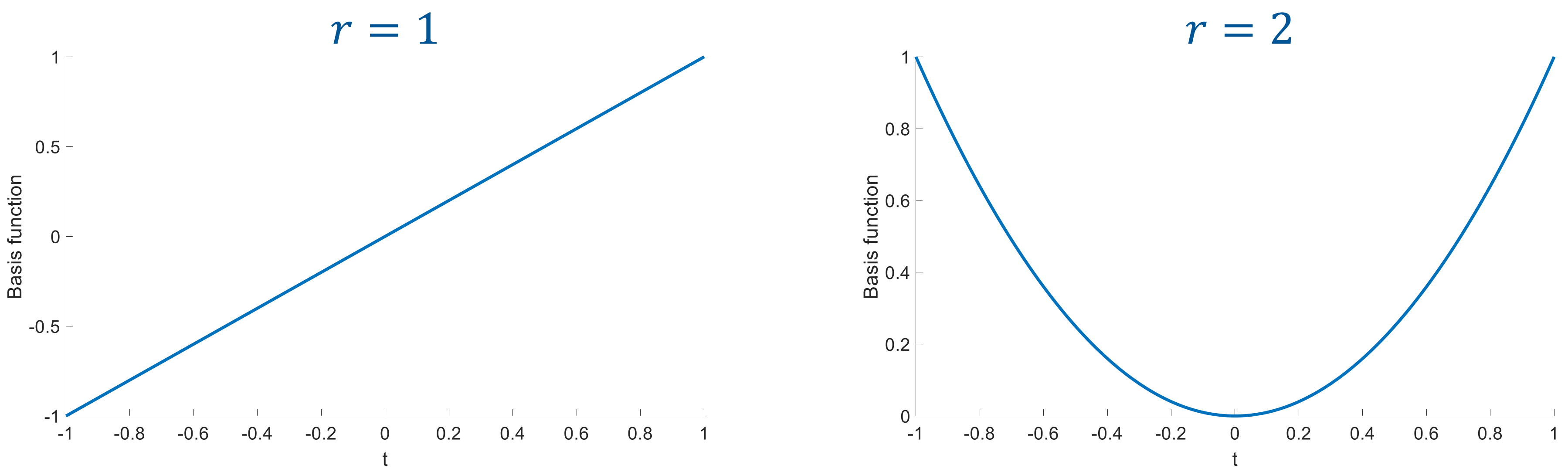
where

$$t = \frac{2x - (x_{\min} + x_{\max})}{x_{\max} - x_{\min}}$$

- All t-values lie in the interval $[-1, 1]$, with $\min\{t_i\} = -1$ and $\max\{t_i\} = 1$

Polynomial calibration Parametrisation [3]

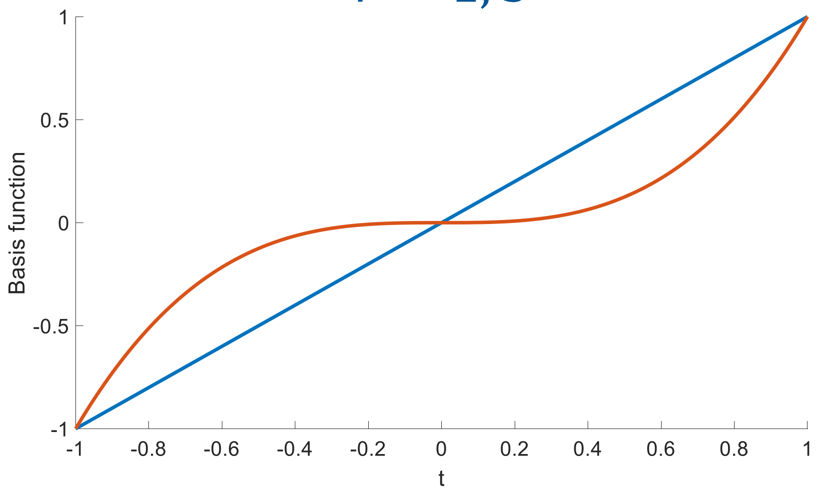
Monomial representation t^r



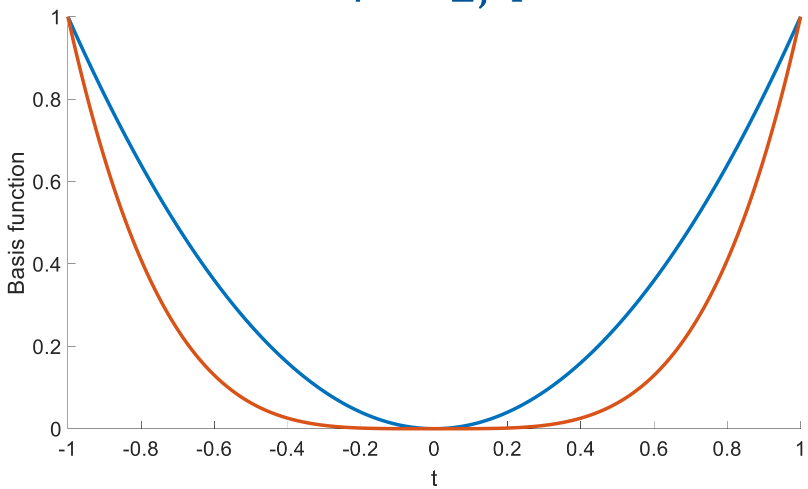
Polynomial calibration Parametrisation [3]

Monomial representation t^r

$r = 1, 3$



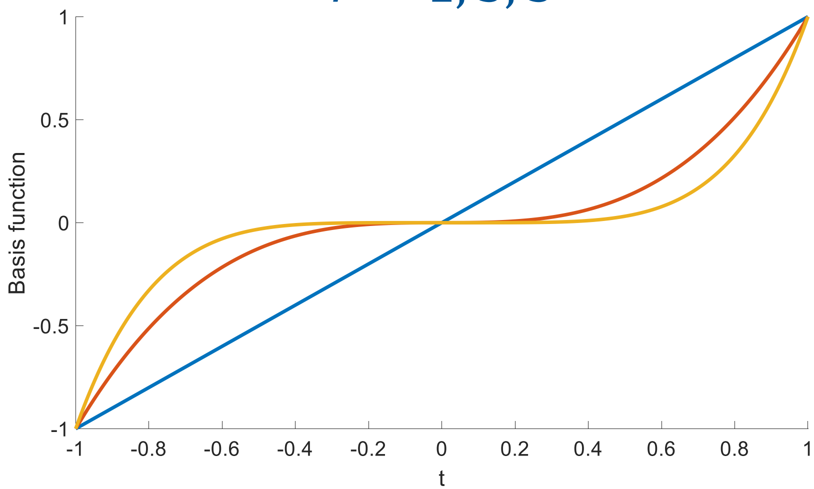
$r = 2, 4$



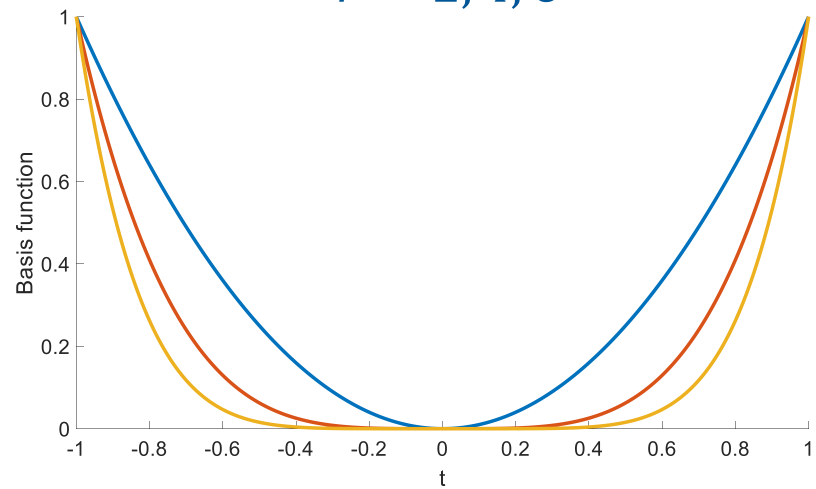
Polynomial calibration
Parametrisation [3]

Monomial representation t^r

$r = 1, 3, 5$



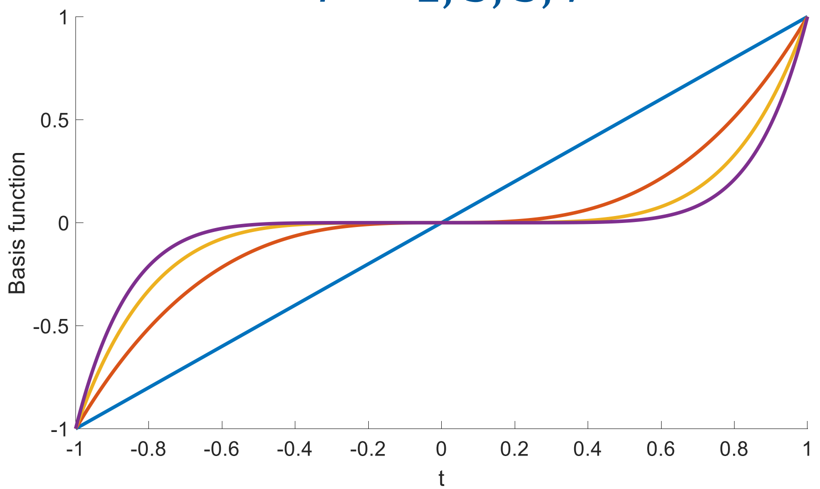
$r = 2, 4, 6$



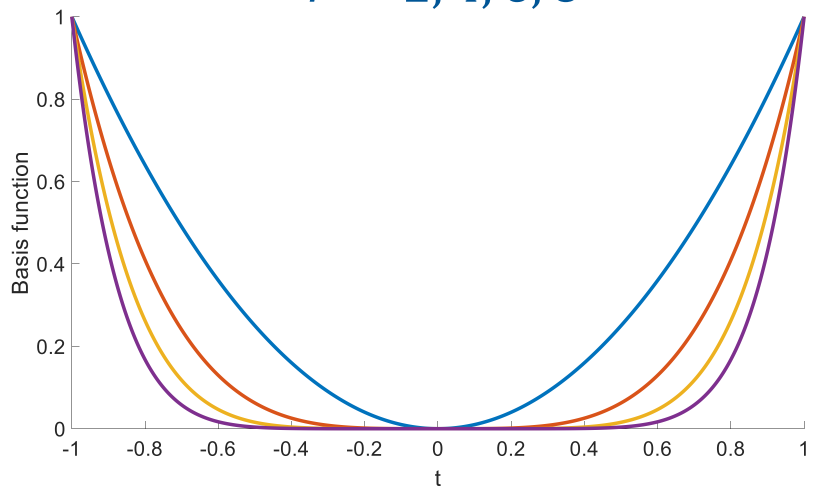
Polynomial calibration Parametrisation [3]

Monomial representation t^r

$r = 1, 3, 5, 7$



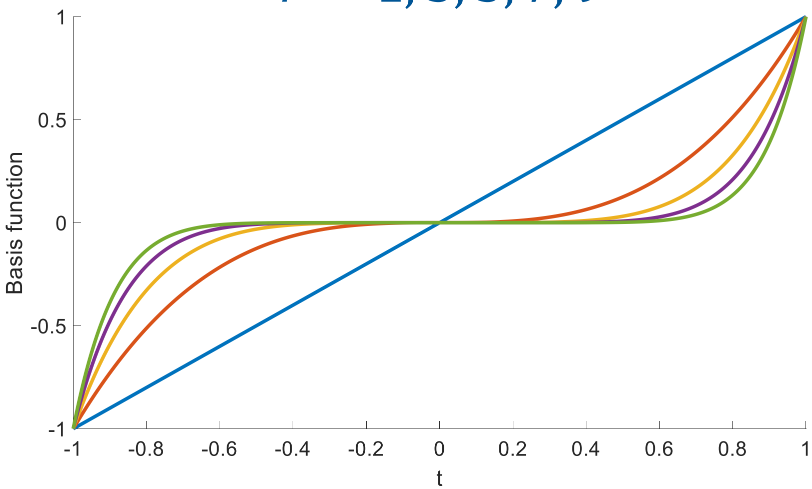
$r = 2, 4, 6, 8$



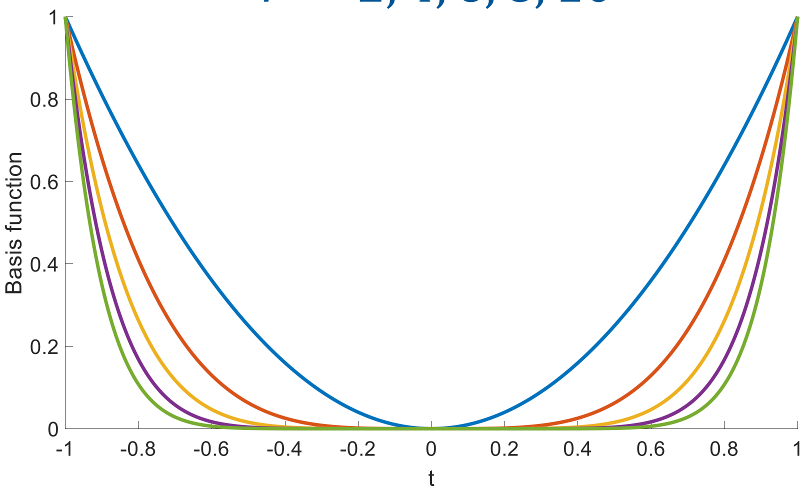
Polynomial calibration Parametrisation [3]

Monomial representation t^r

$r = 1, 3, 5, 7, 9$



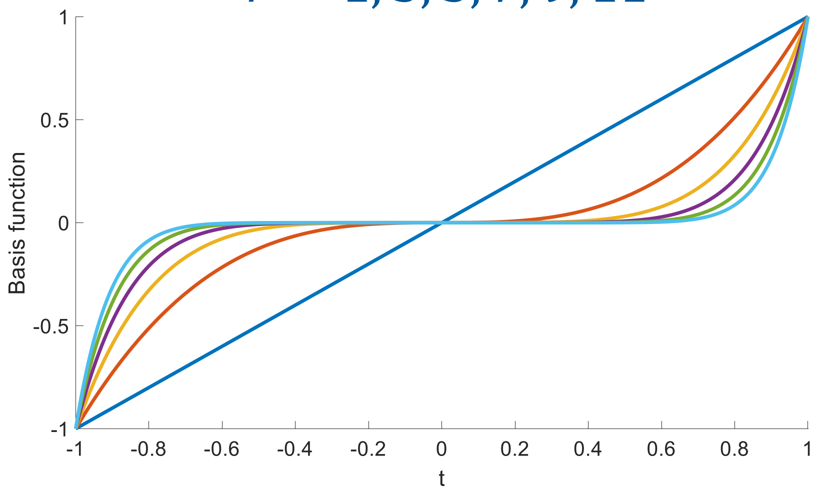
$r = 2, 4, 6, 8, 10$



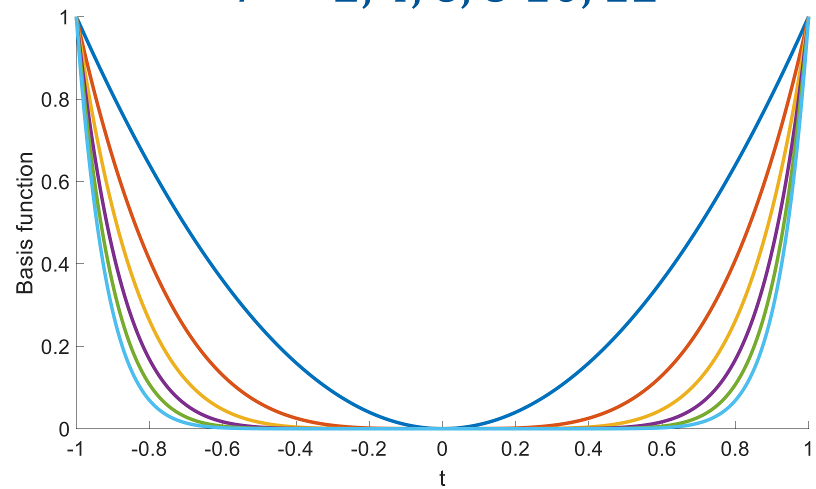
Polynomial calibration Parametrisation [3]

Monomial representation t^r

$r = 1, 3, 5, 7, 9, 11$



$r = 2, 4, 6, 8\ 10, 12$



- Generally fine for low values of n
- Basis functions for large even or odd powers look similar leading to ill-conditioning and loss of numerical precision when determining coefficients

Polynomial calibration
Parametrisation [4]

- Representation in terms of Chebyshev polynomials, i.e.,

$$p(x, \mathbf{D}) = D_0 T_0(t) + D_1 T_1(t) + \cdots + D_n\, T_n(t)$$

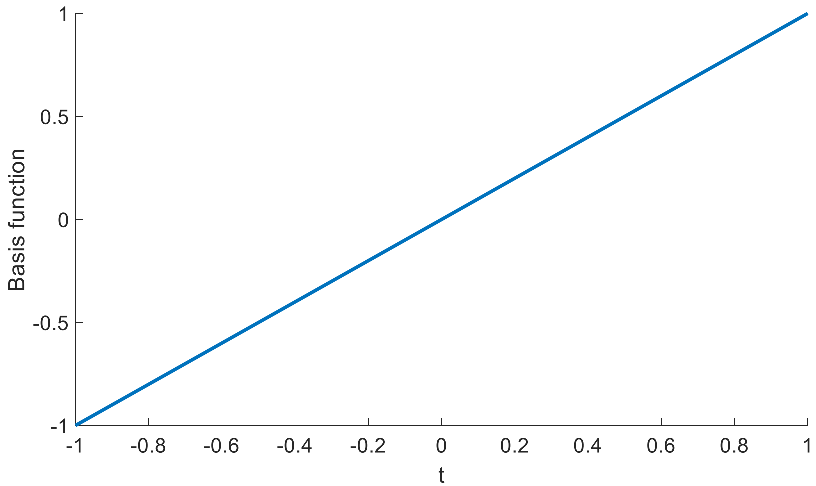
where t is defined as before and

$$T_0(t) = 1,$$
$$T_1(t) = t,$$
$$T_r(t) = 2tT_{r-1}(t) - T_{r-2}(t), r \geq 2$$

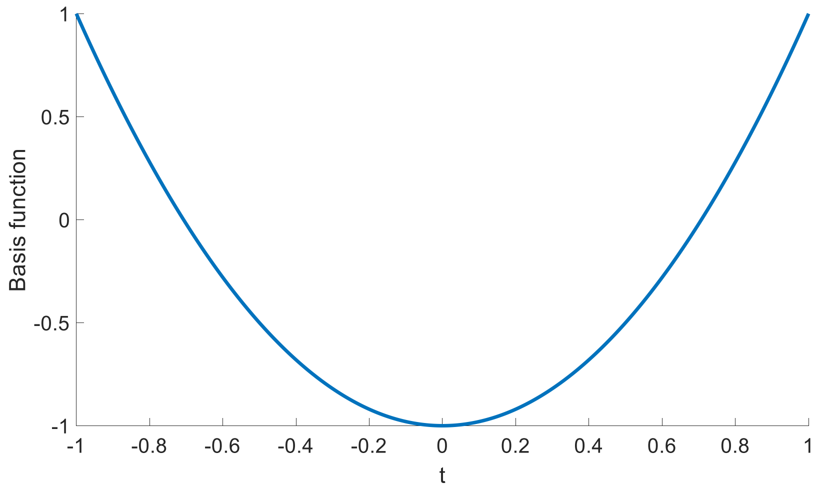
Polynomial calibration Parametrisation [4]

Chebyshev polynomial representation $T_r(t)$

$r = 1$



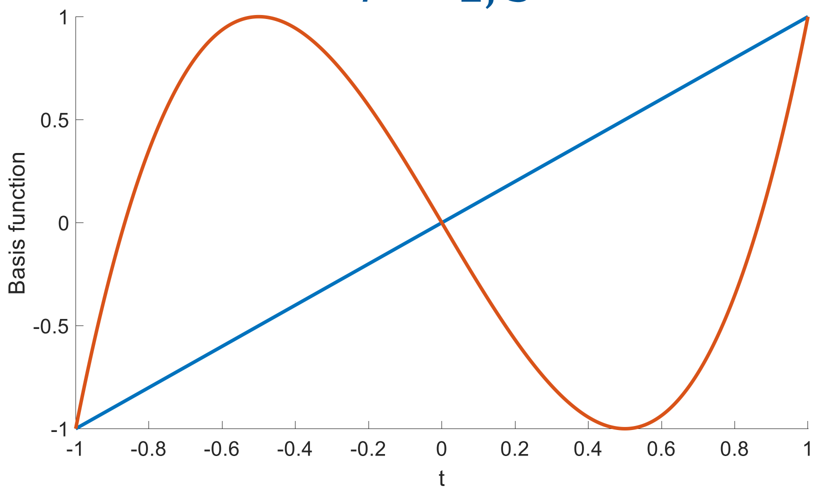
$r = 2$



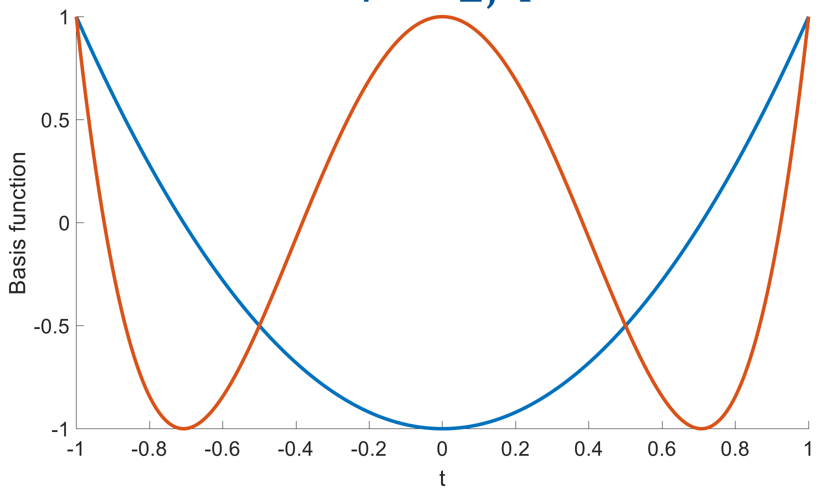
Polynomial calibration
Parametrisation [4]

Chebyshev polynomial representation $T_r(t)$

$r = 1, 3$



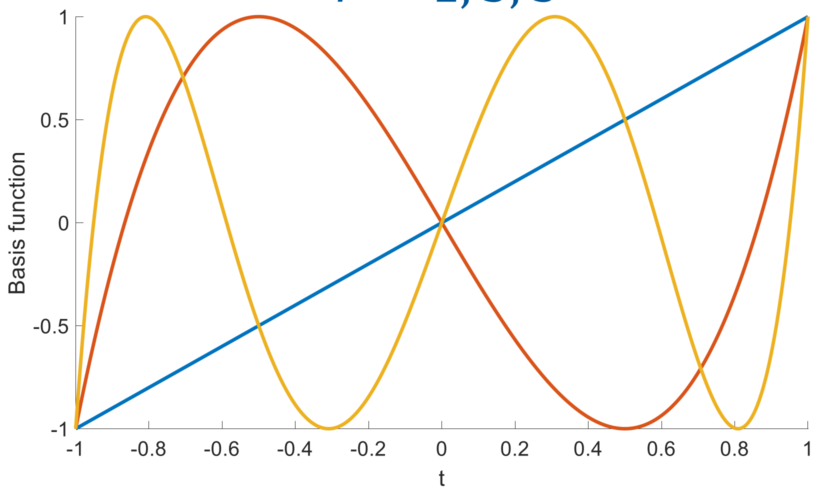
$r = 2, 4$



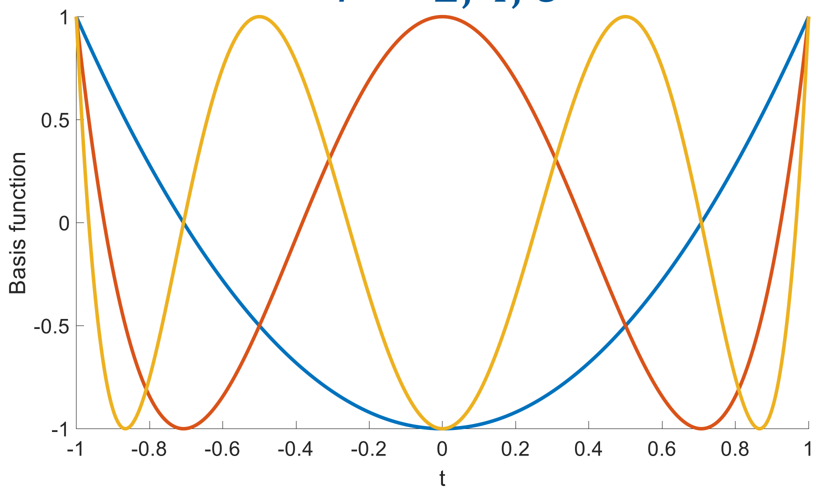
Polynomial calibration
Parametrisation [4]

Chebyshev polynomial representation $T_r(t)$

$r = 1, 3, 5$



$r = 2, 4, 6$



Polynomial calibration
Parametrisation [4]

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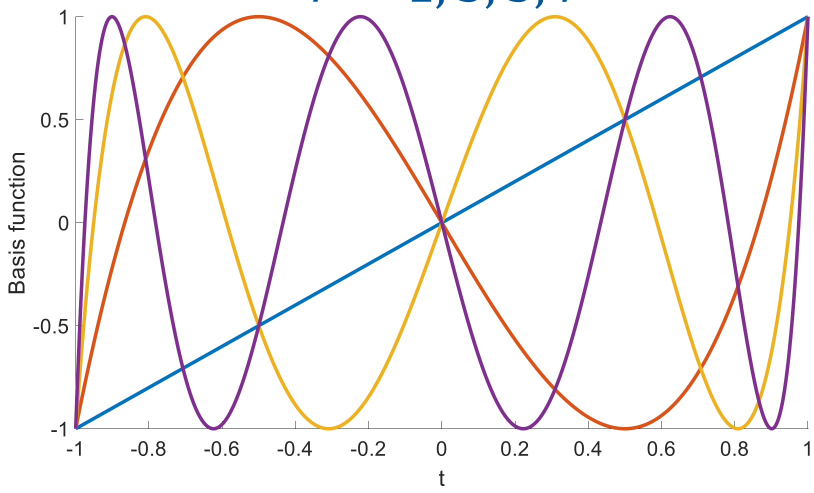
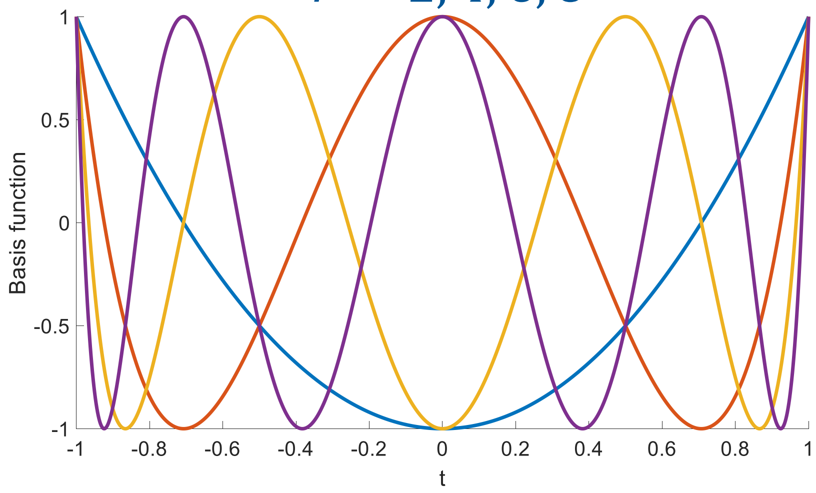


$r = 2, 4, 6, 8$



Polynomial calibration
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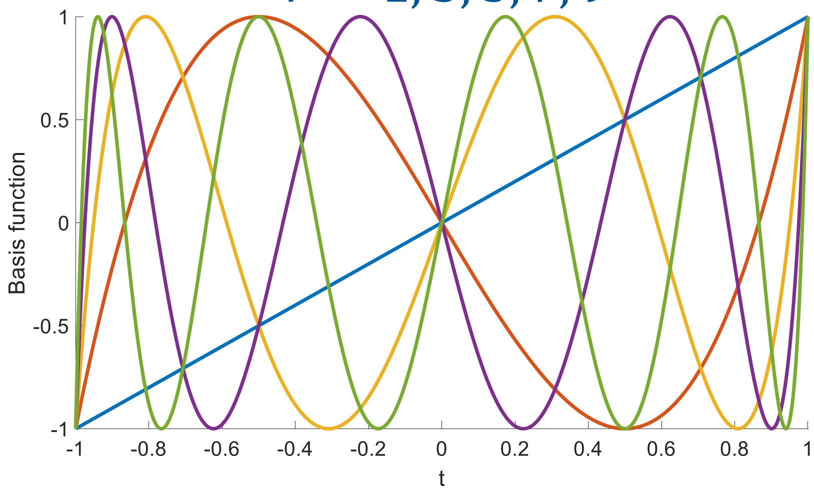
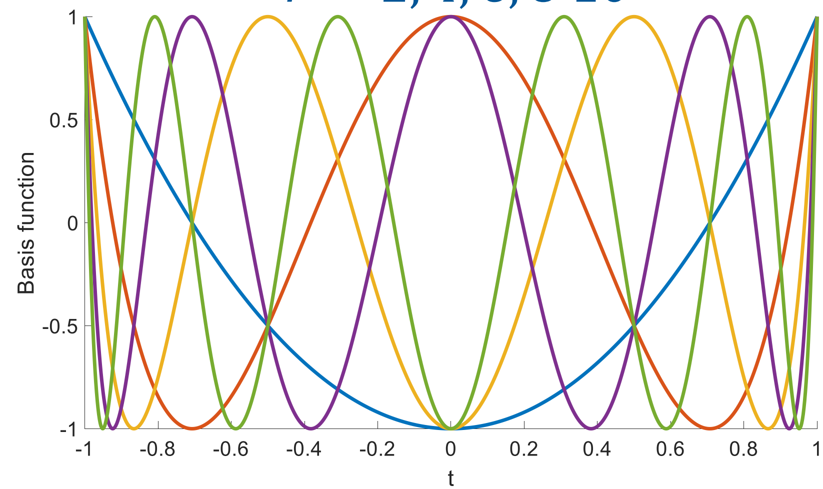


$r = 2, 4, 6, 8\ 10$



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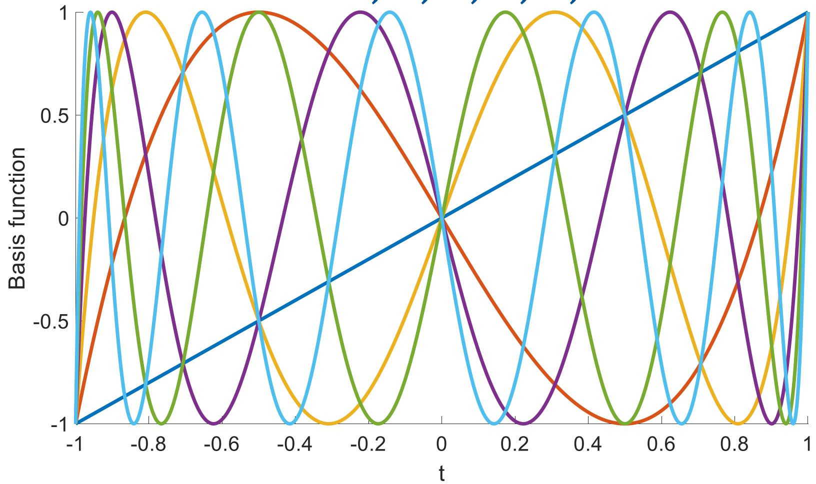

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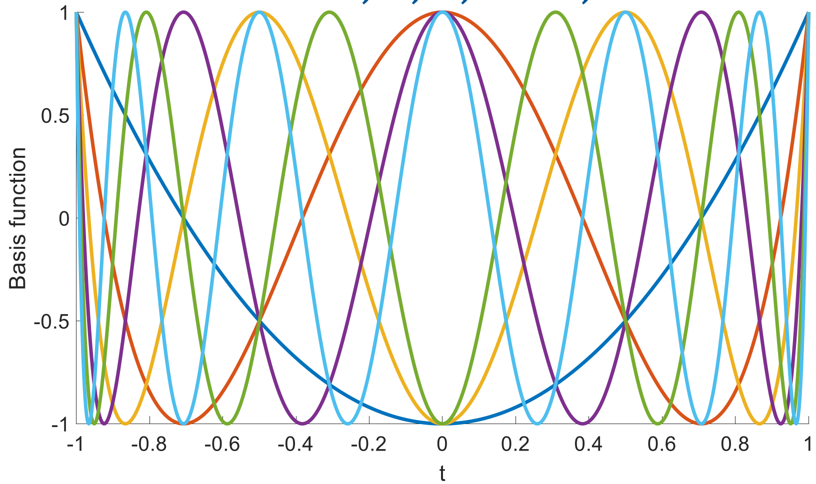

- Basis functions intertwine leading to better numerical conditioning
- Use of Chebyshev polynomials recommended for high values of polynomial degree

Polynomial calibration
Parametrisation

- For numerical reasons, use of Chebyshev polynomials is recommended

- Use of other parametrisations may be fine depending on
  - Nature of data and/or
  - Polynomial degree

Polynomial calibration Parametrisation

- Example: Thermocouple reference function
- Interval $[-50\ °\mathrm{C}, 1064.18\ °\mathrm{C}]$

Degree r	Raw x-values
0	0
1	5.4031×10^{-3}
2	1.2593×10^{-5}
3	-2.3248×10^{-8}
4	3.2203×10^{-11}
5	-3.3147×10^{-14}
6	2.5574×10^{-17}
7	-1.2507×10^{-20}
8	2.7144×10^{-24}

Polynomial calibration Parametrisation

- Example: Thermocouple reference function
- Interval $[-50\ °\mathrm{C}, 1064.18\ °\mathrm{C}]$

Degree r	Raw x-values	Scaled x-values	Normalised	Chebyshev
0	0	0	4.3036	4.6391
1	5.4031×10^{-3}	5.7499	5.5278	5.3711
2	1.2593×10^{-5}	14.2618	0.4784	0.3706
3	-2.3248×10^{-8}	-28.0174	-0.0543	-0.0729
4	3.2203×10^{-11}	41.3005	0.2206	0.0371
5	-3.3147×10^{-14}	-45.2390	-0.1637	-0.0130
6	2.5574×10^{-17}	37.1447	0.0216	0.0022
7	-1.2507×10^{-20}	-19.3310	-0.0249	-0.0004
8	2.7144×10^{-24}	4.4648	0.0252	0.0002

Polynomial calibration Parametrisation

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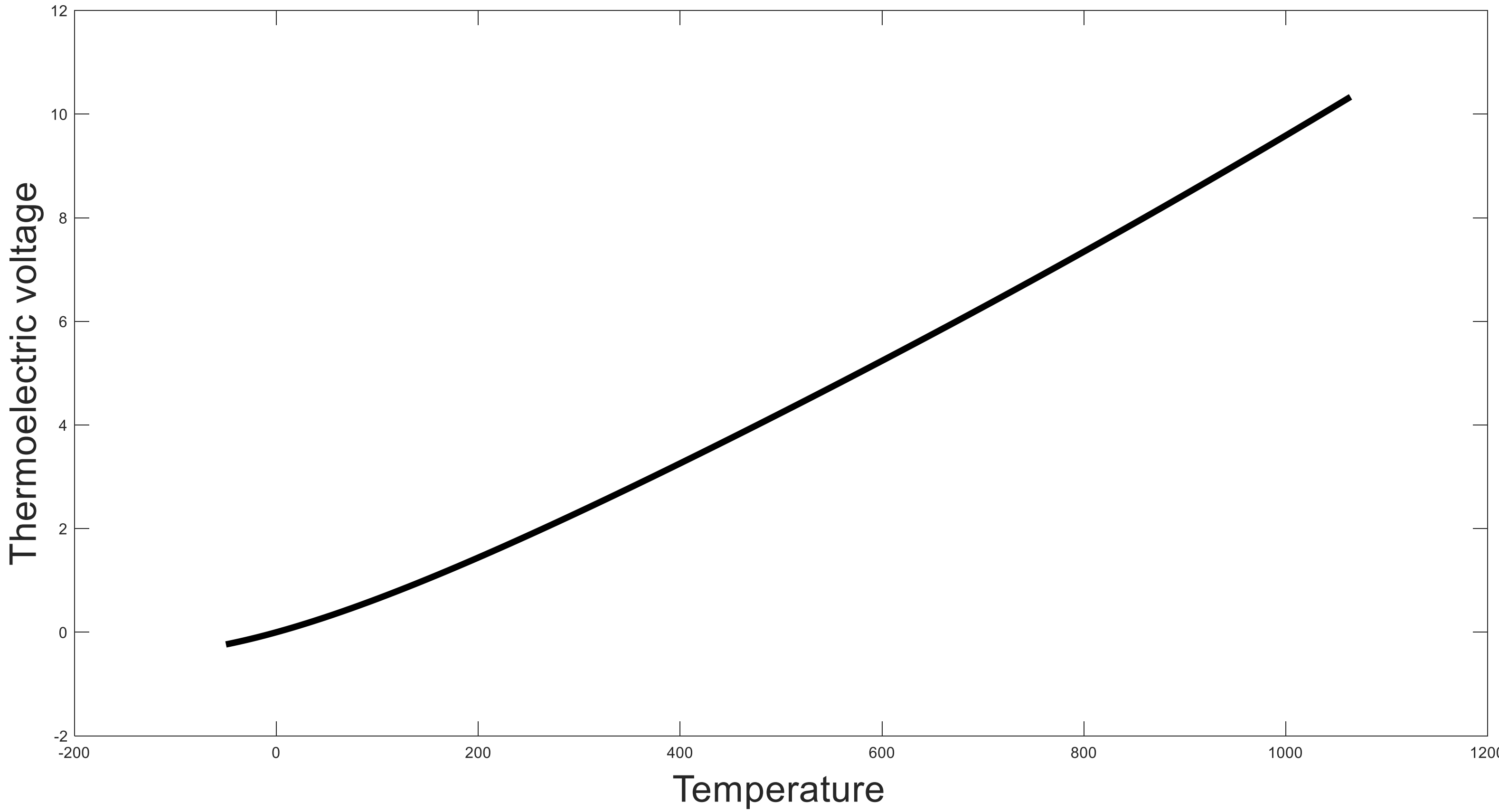

Polynomial degree unknown in advance

- In some metrology applications, the value of polynomial degree is not specified in advance
  - Minimum and/or maximum degree may be specified
- Required therefore to determine calibration functions of different degrees and assess their suitability
- Ideally assessment would be objective rather than subjective

Polynomial degree unknown in advance
Assessment of different degrees:
1. Visual inspection

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- Subjective but can still be useful
- Useful for cases where available data is limited and statistical tests are not so useful
- Suitability (or not) of a particular polynomial degree can be provided by inspection of
  - Plot of measurement data and calibration function
  - Randomness of weighted residuals can be helpful

Polynomial degree unknown in advance
Assessment of different degrees:
2. Monotonicity

- To be useful as a calibration function, a function generally must be strictly monotonic over the interval over which it is defined and to be used

- Simple (but not infallible) approach to check monotonicity
  - Generate large number of uniformly-spaced points over the interval of stimulus values
  - Evaluate calibration function at those points
  - Check if function values form an increasing or decreasing set

- Rigorous approach can be applied for a calibration function expressed in terms of Chebyshev polynomials

Polynomial degree unknown in advance
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Polynomial degree unknown in advance
Assessment of different degrees:
3. Model-selection criteria

- Generic approach
  - Fit polynomial functions of increasing degree
  - For each function, calculate a goodness-of-fit measure
  - Use values of goodness-of-fit measure to select polynomial degree

- A common goodness-of-fit measure is the chi-squared statistic χ^2_{obs}
  - Essentially the sum of squares of weighted residuals

- Other model-selection criteria can be used that provide a balance between goodness of fit and simplicity of model

Polynomial degree unknown in advance
Assessment of different degrees:
3. Model-selection criteria

- Akaike's Information Criterion (AIC)

$$\mathrm{AIC}(n) = \chi^2_{\mathrm{obs}}(n) + 2(n+1)$$

- Corrected AIC (AICc)

$$\mathrm{AICc}(n) = \mathrm{AIC}(n) + \frac{2(n+1)(n+2)}{m-n-2}$$

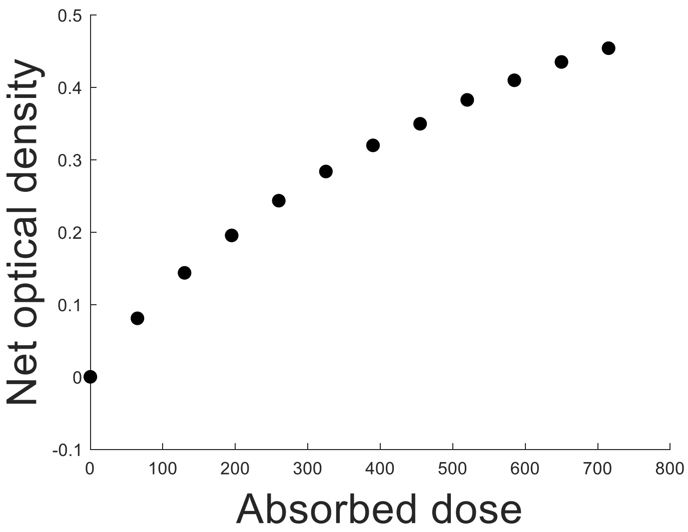
- Bayesian Information Criterion (BIC)

$$\mathrm{BIC}(n) = \chi^2_{\mathrm{obs}}(n) + (n+1)\ln m$$

- For a selected criterion, choose degree that returns the smallest value of that criterion

Polynomial degree unknown in advance
Assessment of different degrees:
3. Model-selection criteria

- Example: Optical density as a function of absorbed dose



Absorbed dose x	Net optical density y	$u(y)$
0	0.0004	0.0017
65	0.0812	0.0016
130	0.1440	0.0017
195	0.1957	0.0020
260	0.2437	0.0020
325	0.2840	0.0024
390	0.3201	0.0024
455	0.3499	0.0026
520	0.3829	0.0026
585	0.4100	0.0029
650	0.4353	0.0029
715	0.4543	0.0031

Polynomial degree unknown in advance
Assessment of different degrees:
3. Model-selection criteria

- Example: Optical density as a function of absorbed dose

Degree n	$\chi^2_{\mathrm{obs}}(n)$	AIC	AICc	BIC
1	1836.5	1840.5	1841.9	1841.5
2	109.5	115.5	118.5	117.0
3	16.2	24.2	30.0	26.2
4	3.0	13.0	23.0	15.4
5	2.7	14.7	31.5	17.6
6	1.3	15.3	43.3	18.7
7	1.0	17.0	65.0	20.9
8	0.8	18.8	108.8	23.2

Polynomial degree unknown in advance
Assessment of different degrees:
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3	16.2	24.2	30.0	26.2
4	3.0	**13.0**	**23.0**	**15.4**
5	2.7	14.7	31.5	17.6
6	1.3	15.3	43.3	18.7
7	1.0	17.0	65.0	20.9
8	0.8	18.8	108.8	23.2

Conclusions

- Numerically stable approaches to determine polynomial calibration functions for different uncertainty structures are well-known
- Various metrology applications require determination of a polynomial calibration function where the polynomial degree is unknown *a priori*
- Approaches that allow suitability of different polynomial degrees to be assessed
  - Visual inspection
  - Monotonicity
  - Model-selection criteria
- Educational issue – understanding of Chebyshev representation

References

- ISO/TS 28038:2018 Determination and use of polynomial calibration functions
- NIST database https://srdata.nist.gov/its90/download/allcoeff.tab