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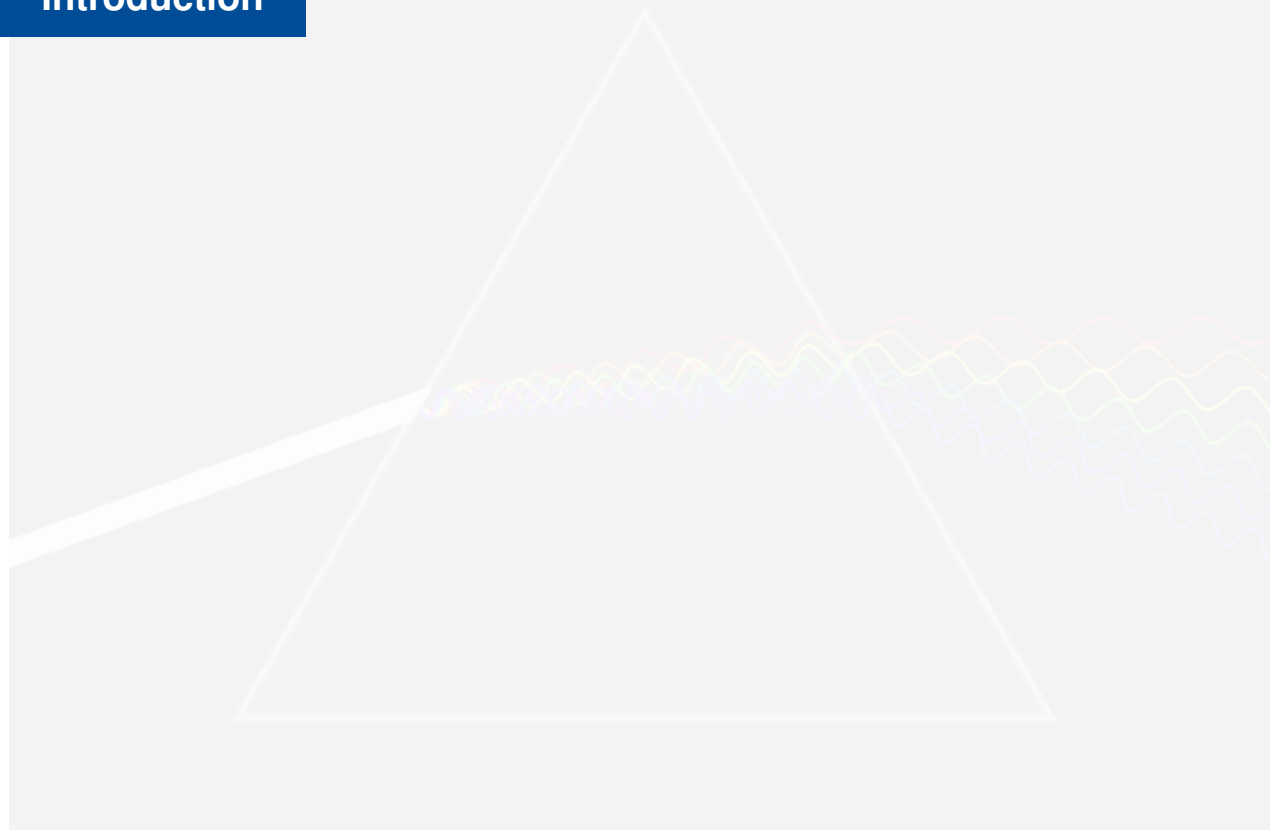
An introduction to spectral methods for solving ODEs

Manuel Borregales

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Post-doc at the Computational Geosciences group, SINTEF Digital, Oslo.*

Numerical methods for ODEs, Karlstad University, 6 Nov 2019.

Introduction



The solution $u(x)$ is **expanded** into a series of **orthogonal functions**.

$$u(x) \approx u^N(x) = \sum_{k=0}^N c_k \phi_k(x)$$



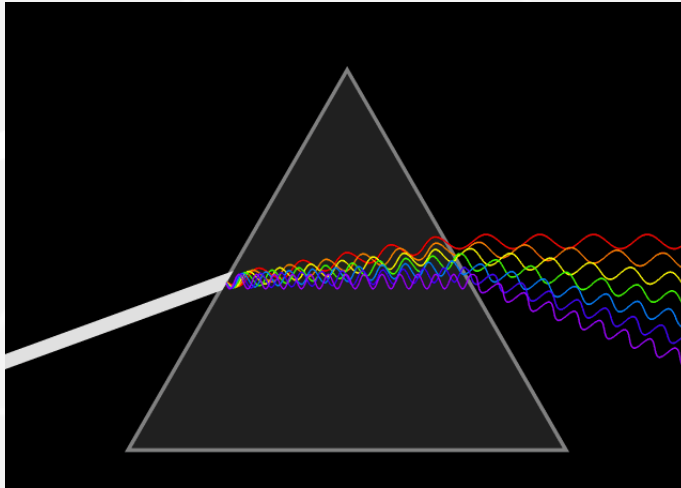
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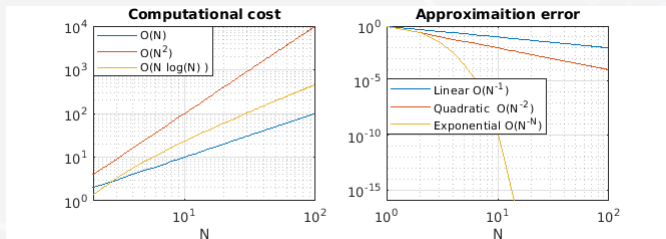
- The numerical solution is related to its spectrum



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- The numerical solution is related to its spectrum
- Exponential convergence rate (Spectral accuracy): $O(h^N), h \approx \frac{1}{N}$
- Computational cost: $O(N \log(N))$



Outline



Introduction

Orthogonal functions

Chebyshev polynomials

Fourier series

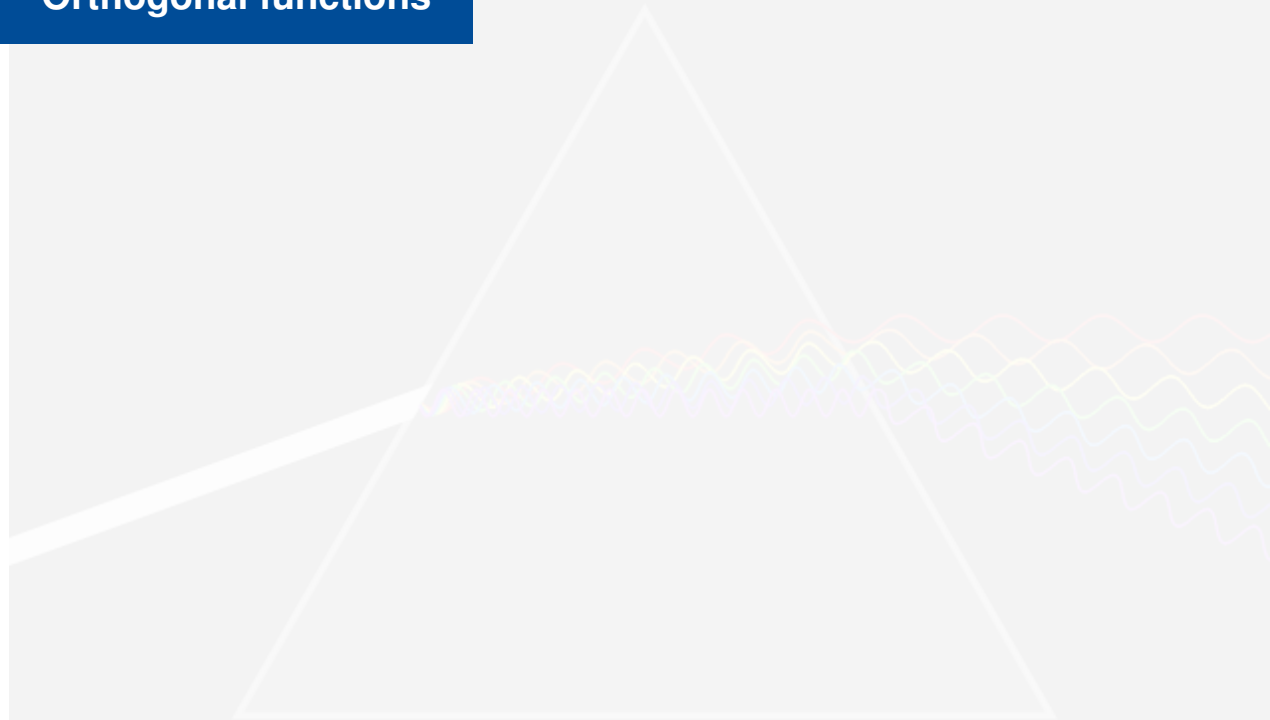
Spectral methods

Conclusion

Recommended references



Orthogonal functions



Orthogonal functions



Two functions $\phi(x)$ and $\varphi(x)$ are orthogonal in an interval $[a, b]$ if

$$\int_a^b \phi(x) \varphi(x) dx = 0$$



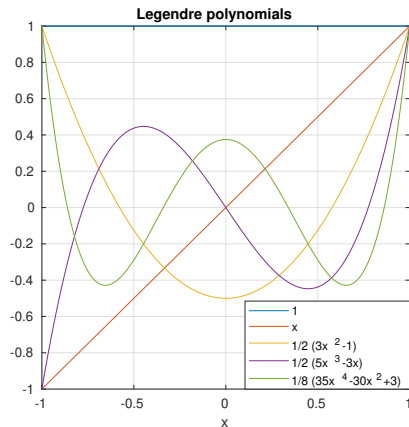
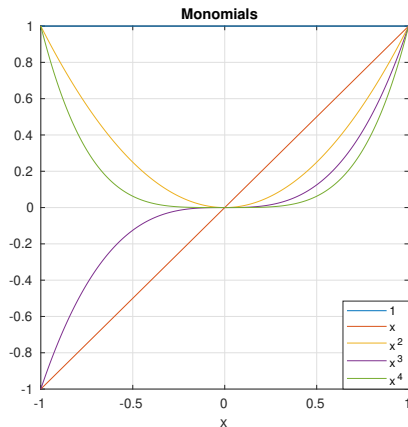
Orthogonal functions



Two functions $\phi(x)$ and $\varphi(x)$ are orthogonal in an interval $[a, b]$ if

$$\int_a^b \phi(x) \varphi(x) dx = 0$$

By applying GramSchmidt process to the basis $\{1, x, x^2, \dots\}$ the Legendre polynomials are obtained.



Orthogonal functions



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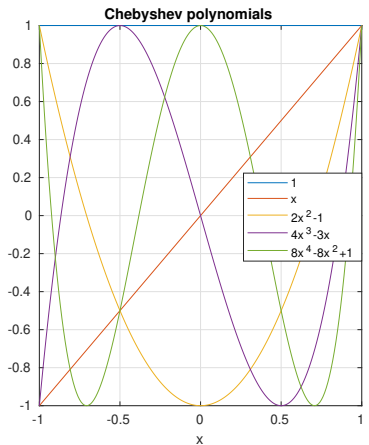
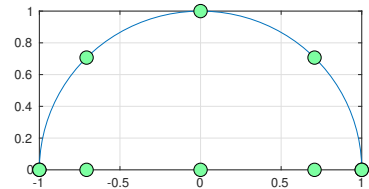
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Chebyshev polynomials of the first kind



- Definition

$$T_n(x) = \cos(n\theta(x)), \quad \theta(x) := \arccos(x)$$



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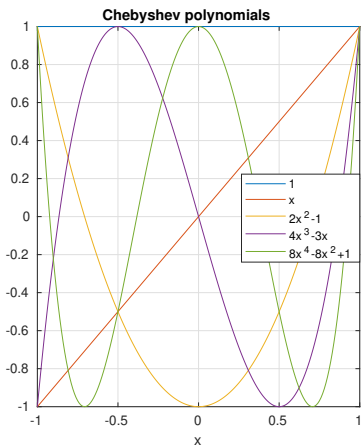
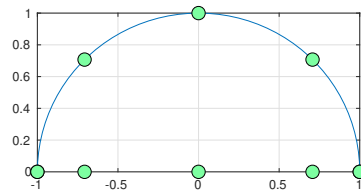
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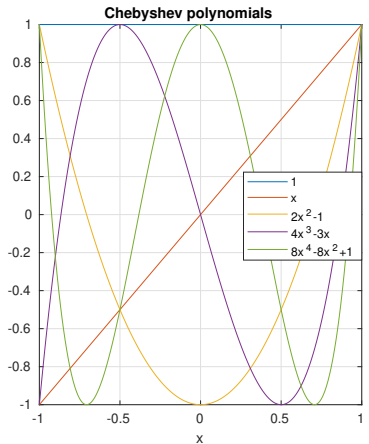
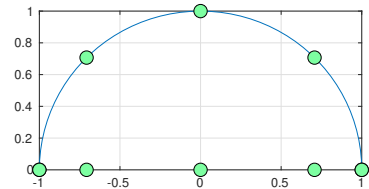
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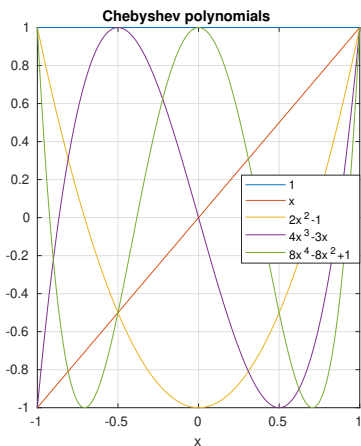
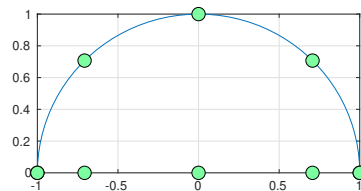
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- Derivatives

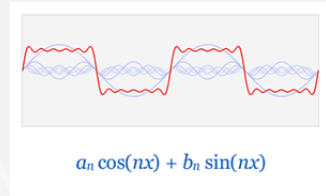
$$\frac{d^p}{dx^p} T_n(x) = \sum_{k=0}^{N-p} D_{n,k,p} T_k(x)$$



Fourier series



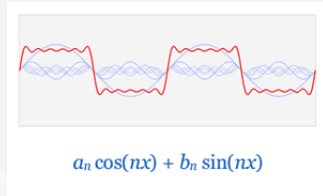
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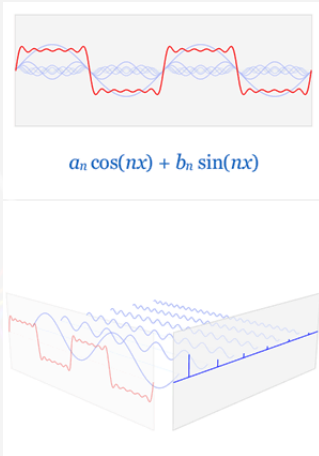


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$$\hat{u}(\xi) = \int_{-\infty}^{\infty} u(x) e^{-i2\pi x \xi} dx$$



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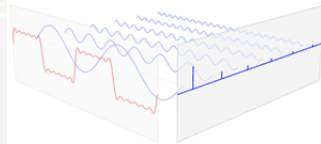
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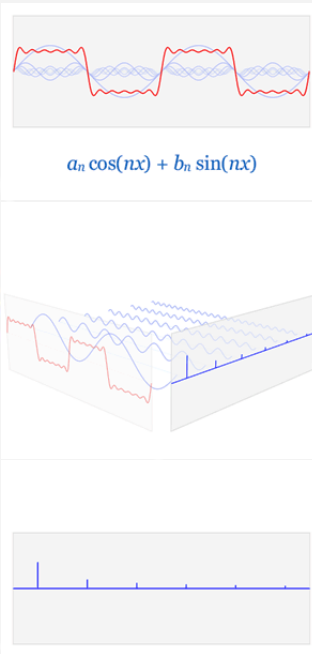
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$$\hat{u}_k = \sum_{n=0}^{N-1} u_n e^{-i2\pi k \frac{n}{N}}$$



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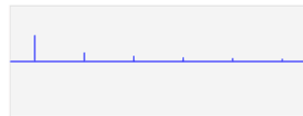
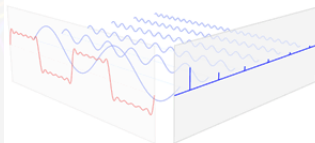
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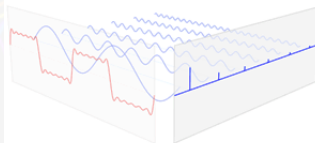
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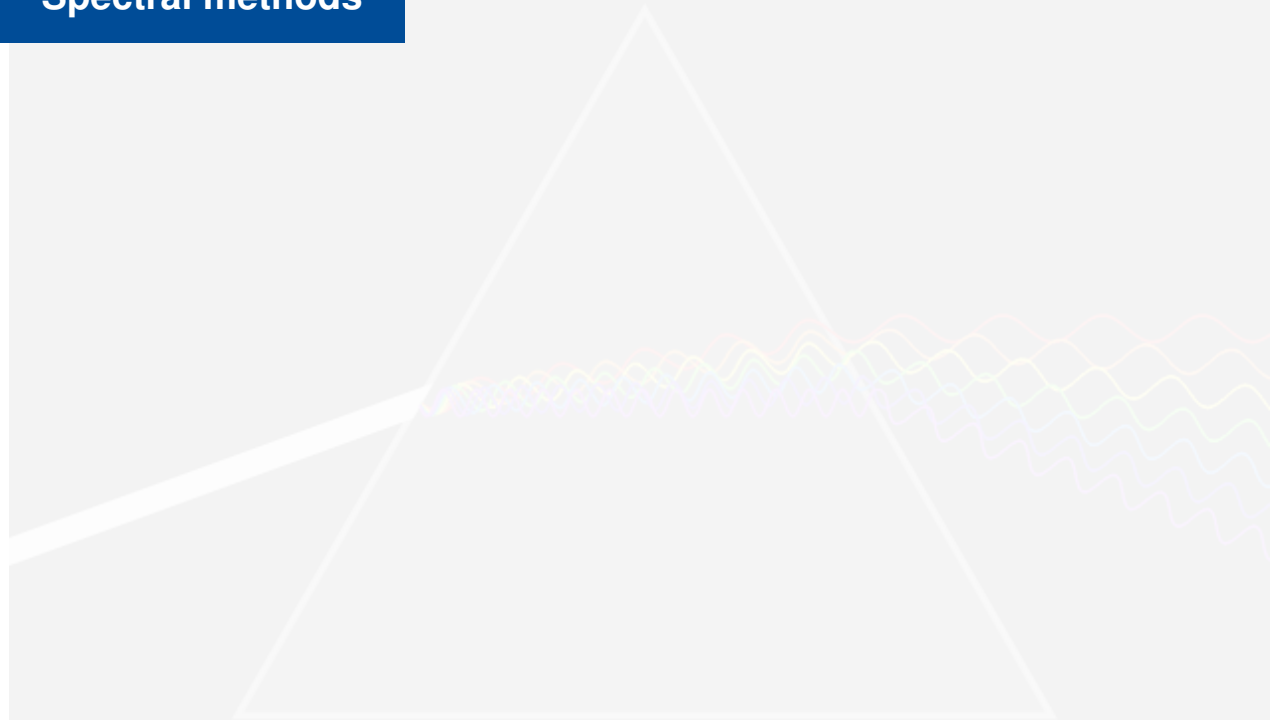
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Spectral methods



$$D u(x) = f(x).$$

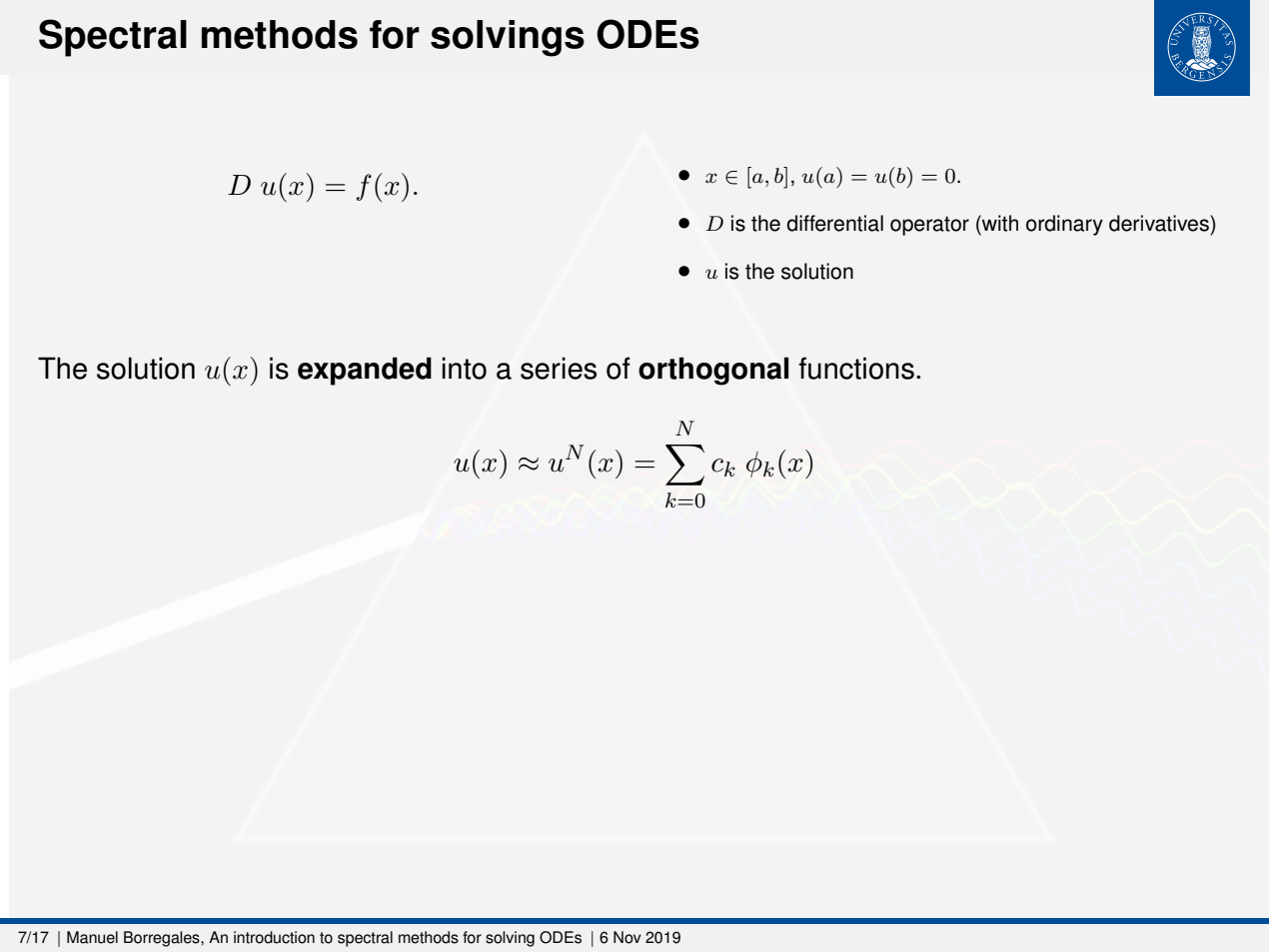
- $x \in [a, b]$, $u(a) = u(b) = 0$.
- D is the differential operator (with ordinary derivatives)
- u is the solution



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The goal of spectral methods is to choose the coefficients c_k such that the residual R is minimized.

$$R(x) := Du^N(x) - f = D \sum_{k=0}^N c_k \phi_k(x) - f(x)$$

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$$R(x_l) = 0, \quad l = 0 : N$$

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Collocation methods: $R(x_l) = 0, \quad l = 0 : N$

Weighted residuals methods: $\int_a^b R(x) \varphi_l(x) w(x) dx = 0, \quad l = 0 : N$

Collocation method (Pseudospectral method)



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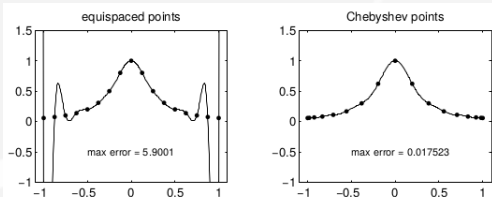


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Create an array of points $\{x_l\}_{l=0}^N$ such that $a = x_0 < x_1 < \dots < x_{N-1} < x_N = b$.

$$u^N(a) = 0, \quad u^N(b) = 0,$$
$$R(x_l) = 0, \quad l = 1 : N - 1.$$



Output 9: Degree N interpolation of $u(x) = 1/(1 + 16x^2)$ in $N + 1$ equispaced and Chebyshev points for $N = 16$. With increasing N , the errors increase exponentially in the equispaced case – the Runge phenomenon – whereas in the Chebyshev case they decrease exponentially.

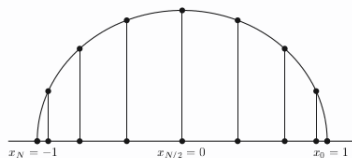


Fig. 5.1. Chebyshev points are the projections onto the x -axis of equally spaced points on the unit circle. Note that they are numbered from right to left.

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$$\sum_{k=0}^N c_k \underline{D\phi_k(x_l)} = f(x_l), \quad l = 1, \dots, N - 1$$

$$\sum_{k=0}^N \underline{(\mathbf{A})_{l,k}} c_k = (\mathbf{b})_l, \quad l = 1, \dots, N - 1$$

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Example

$$D(\cdot) := (\cdot)'' + (\cdot)' + (\cdot), \Rightarrow u'' + u' + u = f(x),$$

$$\sum_{k=0}^N ((\mathbf{D}_2)_{l,k} + (\mathbf{D})_{l,k} + d_l \delta_{lk}) c_k = b_l, \quad l = 1, \dots, N - 1$$

$$(\mathbf{D}_2 + \mathbf{D} + \mathbf{I})c = b$$

Chebyshev

Fourier

$$(\mathbf{D})_{ij} = \begin{cases} \frac{2N^2+1}{6}, & i = j = 0 \\ -\frac{2N^2+1}{6}, & i = j = N \\ -\frac{x_j}{2(1-x_j^2)}, & i = j; 0 \leq j \leq N \\ (-1)^{i+j} \frac{c_j}{c_j(x_i-x_j)}, & i \neq j \end{cases}$$

$$c_j = \begin{cases} 2 & j = 0, N \\ 1 & 1 \leq j \leq N-1 \end{cases}$$

$$(\mathbf{D})_{ij} = \begin{cases} 0 & i = j \\ \frac{1}{2}(-1)^{i-j} \cot\left(\frac{x_i-x_j}{2}\right), & i \neq j \end{cases}$$

$$(\mathbf{D}_2)_{ij} = \begin{cases} -\frac{2N^2+1}{6} & i = j \\ \frac{1}{2}(-1)^{i-j+1} \csc^2\left(\frac{x_i-x_j}{2}\right), & i \neq j \end{cases}$$

$$(\mathbf{D}_k) = (\mathbf{D})^k$$

the kth differentiation matrix will be the same as applying the first differentiation matrix k times

⁰D. Gottlieb, M. Y. Hussaini, and S. A. Orszag. [Introduction: Theory and Applications of Spectral Methods](#). *Spectral Methods for Partial Differential Equations*. SIAM, 1984.

Collocation method (Pseudospectral method)



Fourier + Fast Fourier Transform

Example

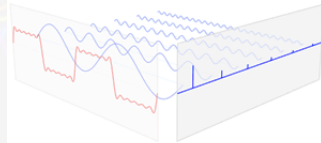
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$$\phi_k(x) = e^{ikx}$$



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Collocation method (Pseudospectral method)



Fourier + Fast Fourier Transform

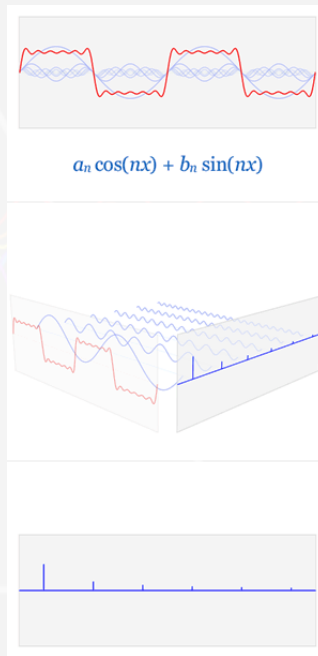
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$$\sum_{k=0}^N c_k \phi_k''(x_l) = f(x_l), \quad l = 1, \dots, N-1$$

$$\phi_k(x) = e^{ikx}$$

$$\sum_{k=0}^N c_k (ik)^2 e^{ikx} = f(x_l), \quad l = 1, \dots, N-1$$



Collocation method (Pseudospectral method)



Fourier + Fast Fourier Transform

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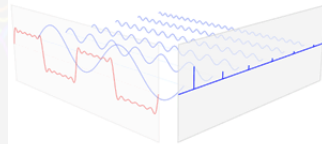
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$$\mathcal{F} \left\{ \sum_{k=0}^N c_k (ik)^2 e^{ikx} \right\} = \mathcal{F} \{ f(x_l) \}, \quad l = 1, \dots, N-1$$



$$a_n \cos(nx) + b_n \sin(nx)$$



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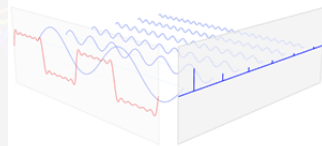
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$$c_k (ik)^2 = \hat{f}_l \rightarrow c_k = \frac{\hat{f}_l}{(ik)^2}$$



$$a_n \cos(nx) + b_n \sin(nx)$$



$$\int_a^b R(x) \varphi_l(x) w(x) dx = 0, \quad l = 0, \dots, N$$

Boundary conditions $\phi_k(a) = \phi_k(b) = 0, \quad k = 0, \dots, N$

$$\sum_{k=0}^N \left(\int_a^b \underline{D(\phi_k(x)) \phi_l(x) w(x) dx} \right) c_k = \int_a^b f(x) \phi_l(x) w(x) dx, \quad l = 0 \dots N$$

$$\sum_{k=0}^N \underline{(\mathbf{A})_{l,k}} c_k = (\mathbf{b})_l, \quad l = 0, \dots, N$$

$$\mathbf{A} \mathbf{c} = \mathbf{b}$$

Example

$$D(\cdot) := (\cdot)'' + (\cdot)' + (\cdot), \Rightarrow \quad u'' + u' + u = f(x),$$

$$\sum_{k=0}^N ((\mathbf{D}_2)_{l,k} + (\mathbf{D})_{l,k} + d_l \delta_{lk}) c_k = \mathbf{b}_l, \quad l = 0, \dots, N$$

$$(\mathbf{D}_2 + \mathbf{D} + \mathbf{I}) \mathbf{c} = \mathbf{b}$$

Collocation method vs Galerkin method



Collocation method

$$u^N(a) = 0, u^N(b) = 0,$$
$$R(x_l) = 0, l = 1 : N - 1$$

Galerkin method

$$\int_a^b R(x) \varphi_l(x) w(x) dx = 0, l = 1 : N - 1$$

$$\varphi_l \in \text{span}\{\{\phi_k\}_{k=0}^N\}$$

$$\underline{(\mathbf{A})}_{l,k} = \int_a^b D(\phi_k(x)) \varphi_l(x) w(x) dx$$

Methods

$$\sum_{k=0}^N c_k \underline{D\phi_k(x_l)} = f(x_l), l = 1, \dots, N - 1$$

$$(\mathbf{b})_l = \int_a^b f(x) \varphi_l(x) w(x) dx, l = 0 \dots N$$

$$\sum_{k=0}^N \underline{(\mathbf{A})}_{l,k} c_k = (\mathbf{b})_l, l = 1, \dots, N - 1$$

$$\sum_{k=0}^N \underline{(\mathbf{A})}_{l,k} c_k = (\mathbf{b})_l, l = 0, \dots, N$$

$$\mathbf{A}c = \mathbf{b}$$

$$\mathbf{A}c = \mathbf{b}$$

- 1) Dense matrix **A**
- 2) No integration need it
- 3) Easy to implement
- 4) BC are imposed in the algebraic system

- 1) Banded matrix **A**
- 2) Requires integration for the right hand side
- 3) Slightly higher accuracy
- 4) BC are imposed in the trial functions

$$\int_a^b R(x) \varphi_l(x) w(x) dx = 0, \quad l = 0, \dots, N$$

$$\int_a^b \left(D \sum_{k=0}^N c_k \phi_k(x) - f(x) \right) \varphi_l(x) w(x) dx = 0$$

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Trial and test function $\{\phi_k\}_{k=0}^N, \{\varphi_l\}_{l=0}^N$

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Trial and test function $\{\phi_k\}_{k=0}^N, \{\varphi_l\}_{l=0}^N$

- Collocation

Orthogonality $w(x)$

- Legendre polynomials $P_l^m(x)$
- Laguerre polynomials $L_k(x)$
- Hermite polynomials $H_k(x)$
- Chebyshev polynomials $T_k(x)$
- Trigonometric functions e^{ikx} (Fourier)

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- Collocation
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- Petrov-Galerkin $\{\phi_k\}_{k=0}^N \neq \{\varphi_l\}_{l=0}^N$

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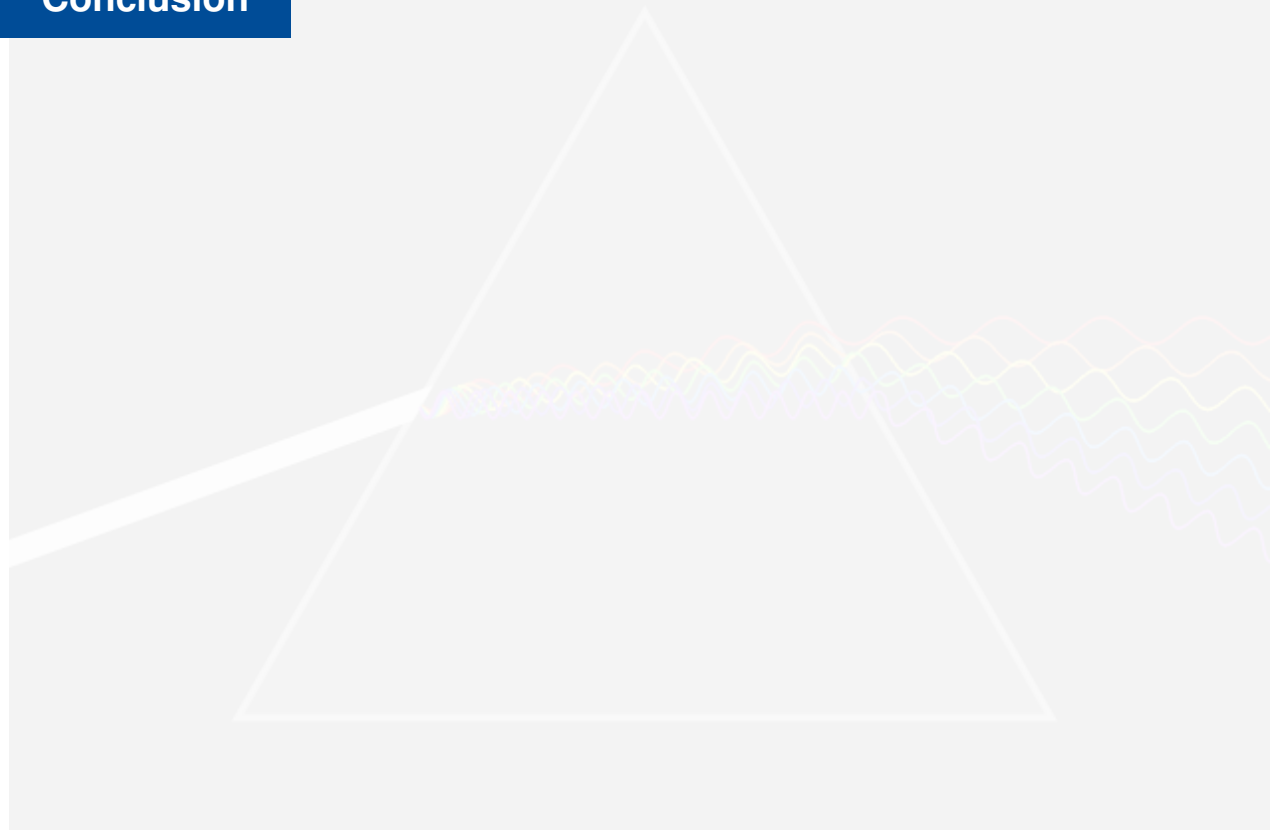
Trial and test function $\{\phi_k\}_{k=0}^N, \{\varphi_l\}_{l=0}^N$

- Collocation
- Galerkin $\{\phi_k\}_{k=0}^N = \{\varphi_l\}_{l=0}^N$
- Tau-Lanczos $\{\phi_k\}_{k=0}^N = \{\varphi_l\}_{l=0}^N$
- Petrov-Galerkin $\{\phi_k\}_{k=0}^N \neq \{\varphi_l\}_{l=0}^N$
- Least square $\{\phi_k\}_{k=0}^N, \{\varphi_l\}_{l=0}^M$ with $N \neq M$

Orthogonality $w(x)$

- Legendre polynomials $P_l^m(x)$
- Laguerre polynomials $L_k(x)$
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- Trigonometric functions e^{ikx} (Fourier)

Conclusion



Recommended references



- D. Dutykh, [A brief introduction to pseudo-spectral methods: application to diffusion problems](#), *Lecture notes*, 38 pp, 2016. CNRSLAMA, Universit Savoie Mont Blanc, France arXiv:1606.05432v2 [math.NA] 14 Feb 2019
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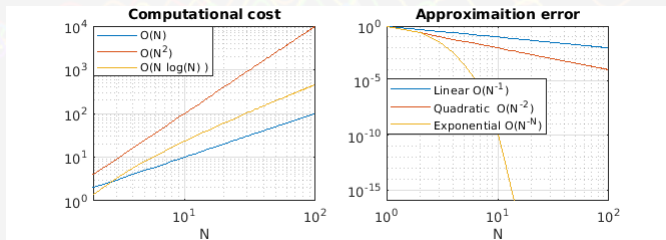


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- M.M. Khader, S. Mziou **Chebyshev spectral method** for studying the viscoelastic slip flow due to a permeable stretching surface embedded in a **porous medium** with viscous dissipation and non-uniform heat generation. *Boundary Value Problems* , (37) 2017.
- V. Vaibhav A **Fast Chebyshev Spectral Method** for Nonlinear Fourier Transform arXiv:1909.03710 [physics.comp-ph] Submitted on 9 Sep 2019)

- Spectral methods are a family of methods where the solution of a ODE u is **expanded** into a series of **orthogonal** functions
- The numerical solution is related to its spectrum



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- Spectral accuracy: $O(h^N), h \approx \frac{1}{N}$
- Computational cost: $O(N \log N)$

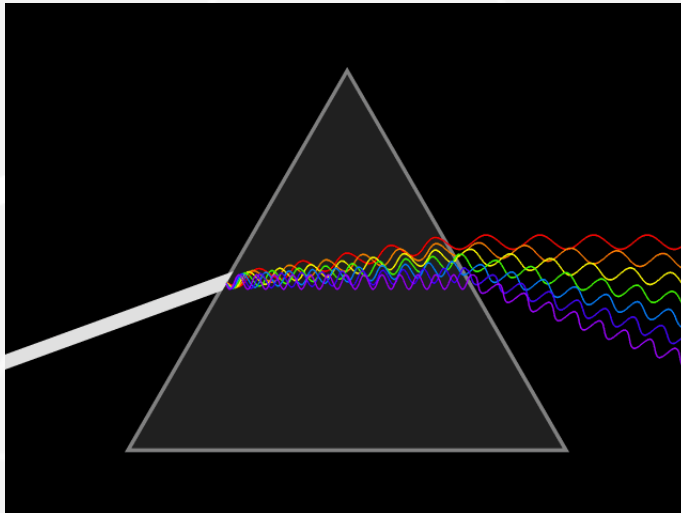


Conclusion



- Spectral methods are a family of methods where the solution of a ODE u is **expanded** into a series of **orthogonal** functions
- The numerical solution is related to its spectrum
- Spectral accuracy: $O(h^N)$, $h \approx \frac{1}{N}$
- Computational cost: $O(N \log N)$
- The examples and the slides are available in GitHub <https://github.com/tayloris/spectral.git>

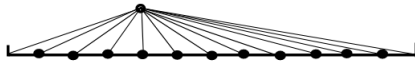
Thanks for your attention



1.4 Comparisons with Finite Difference Method: Why Spectral Methods are Accurate and Memory-Minimizing

Finite difference methods approximate the unknown $u(x)$ by a sequence of overlapping polynomials which interpolate $u(x)$ at a set of grid points. The derivative of the local interpolant is used to approximate the derivative of $u(x)$. The result takes the form of a weighted sum of the values of $u(x)$ at the interpolation points.

Spectral
One high-order polynomial for WHOLE domain



Finite Difference
Multiple Overlapping Low-Order Polynomials



Finite Element/Spectral Element
Non-Overlapping Polynomials, One per Subdomain

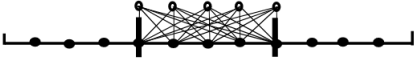


Figure 1.3: Three types of numerical algorithms. The thin, slanting lines illustrate all the grid points (black circles) that *directly* affect the estimates of derivatives at the points shown above the lines by open circles. The thick black vertical lines in the bottom grid are the subdomain walls.

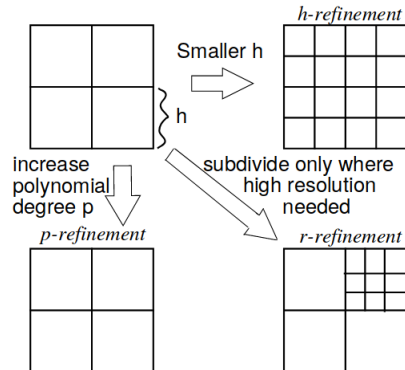


Figure 1.2: Schematic of three types of finite elements

¹J. P. Boyd. *Chebyshev and Fourier spectral methods*. Dover Pubns, 2001.

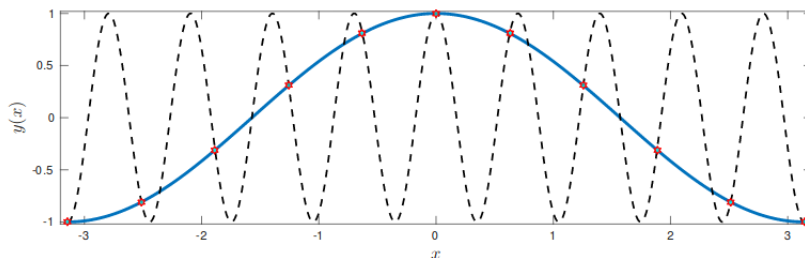


Figure 4. Illustration of the aliasing phenomenon: two FOURIER modes are indistinguishable on the discrete grid. The modes represented here are $\cos(x)$ and $\cos(9x)$ and the discrete grid is composed of $N = 11$ equispaced points on the segment $[-\pi, \pi]$.