

Numerical Methods

Polynomial and Fourier Approximation

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Overview of Approximation theory

Data approximation Given data points $(x_1, y_1), \dots, (x_m, y_m)$, find a function g such that the points (x_i, y_i) satisfy $y_i \approx g(x_i)$.

Function approximation Given a function $f : [a, b] \rightarrow \mathbb{R}$, find a simpler function g such that $g(x) \approx f(x)$.

Approximating functions Choose an appropriate class of approximating functions.
e.g. polynomials, cubic splines, trigonometric functions.

Quality of approximation Choose an appropriate measure of the quality of the approximation.

e.g. Uniform polynomial approximation Given a continuous function f defined on $[a, b]$, find a polynomial function g of degree n minimising

$$\|g - f\|_{\infty} = \max_{x \in [a, b]} |g(x) - f(x)|$$

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Least squares data approximation

Least-squares criterion Choose an approximating function g minimising the *sum-of-squares* error

$$E_2 = \sum_{i=1}^m (g(x_i) - y_i)^2.$$

Root mean-square error The *mean-square* error is $\frac{1}{m} \sum_{i=1}^m (g(x_i) - y_i)^2$.

The *root-mean-square* error is

$$\sqrt{\frac{1}{m} \sum_{i=1}^m (g(x_i) - y_i)^2}.$$

Rationale Least-squares:

- Is statistically optimal if the y_i are subject to a normally-distributed measurement error.
- Provides a good balance between small and large errors.
- Is mathematically easy to work with.

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Least squares variants

Weighted least squares Minimise $\sum_{i=1}^m w_i (g(x_i) - y_i)^2$ where each $w_i > 0$.

Linear regression Approximate by $g(x) = \sum_{j=0}^n a_j \phi_j(x)$, a linear combination of (usually *nonlinear*) *basis* functions ϕ_j .

Obtain a *linear* system for the coefficients.

Polynomial approximation Approximate by a polynomial p .

In practise, better to use a different basis than functions x^j !

Nonlinear least squares If the approximating functions are not linear in the *coefficients* a_i e.g. $g(x) = a_0 \exp(a_1 x)$, obtain nonlinear equations for the best fit.

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Least-squares function approximation

Function approximation Given $f : [a, b] \rightarrow \mathbb{R}$, find a function g approximating f minimising error

$$E = \int_a^b (g(x) - f(x))^2 dx.$$

Weighted function approximation Minimise with respect to a weight $w(x) > 0$, with error

$$E = \int_a^b w(x)(g(x) - f(x))^2 dx.$$

Weighted root-mean-square error The *weighted root-mean-square error* is

$$\sqrt{\frac{\int_a^b w(x)(g(x) - f(x))^2 dx}{\int_a^b w(x) dx}}.$$

If $|g(x) - f(x)| \in [\underline{b}, \bar{b}]$ for all x , then the weighted root-mean-square error also lies in $[\underline{b}, \bar{b}]$.

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Discrete Least Squares

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Linear least squares

Linear least squares Take $g(x) = a_1x + a_0$. Minimise

$$E_2(a_0, a_1) = \sum_{i=1}^m (a_1x_i + a_0 - y_i)^2.$$

To find a_0 and a_1 minimising $E_2(a_0, a_1)$, require

$$\frac{\partial E_2}{\partial a_0} = \sum_{i=1}^m 2(a_1x_i + a_0 - y_i) = 0;$$

$$\frac{\partial E_2}{\partial a_1} = \sum_{i=1}^m 2x_i(a_1x_i + a_0 - y_i) = 0.$$

Rearranging gives

$$a_0 \sum_{i=1}^m x_i + a_1 \sum_{i=1}^m x_i^2 = \sum_{i=1}^m x_i y_i;$$

$$a_0 m + a_1 \sum_{i=1}^m x_i = \sum_{i=1}^m y_i.$$

This is a linear equation!

Define averaged quantities $\overline{X} = \frac{1}{m} \sum_{i=1}^m x_i$ etc.

Obtain

$$a_0 \overline{X} + a_1 \overline{X^2} = \overline{XY}; \quad a_0 + a_1 \overline{X} = \overline{Y}.$$

This simplifies to

$$a_1 = \frac{\overline{XY} - \overline{X}\overline{Y}}{\overline{X^2} - \overline{X}^2}; \quad a_0 = \overline{Y} - a_1 \overline{X}.$$

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Linear least squares

Example Fit a linear function to data

x_i	0.0	0.2	0.3	0.7	1.0
y_i	0.39	0.56	0.64	0.89	0.99

Compute

						sum	av
x_i	0.0	0.2	0.3	0.7	1.0	2.2	0.44
y_i	0.39	0.56	0.64	0.89	0.99	3.47	0.694
x_i^2	0.00	0.04	0.09	0.49	1.00	1.62	0.324
$x_i y_i$	0.000	0.1120	0.192	0.623	0.990	1.917	0.3834

So

$$a_1 = \frac{\overline{XY} - \overline{X}\overline{Y}}{\overline{X^2} - \overline{X}^2} = \frac{0.3834 - 0.44 \times 0.694}{0.324 - 0.44^2} = \frac{0.07804}{0.1304} = 0.59847(5dp);$$

$$a_0 = \overline{Y} - a_1 \overline{X} = 0.694 - 0.59847 \times 0.44 = 0.43067(5dp).$$

Least-squares approximant $g(x) = a_0 + a_1 x = 0.43067 + 0.59847x$.

Approximate $y(0.5) \approx g(0.5) = 0.72991 = 0.73(2dp; \text{precision of data})$.

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Linear least-squares regression

Linear regression Take $g(x) = \sum_{j=0}^n a_j \phi_j(x)$. Minimise

$$E_2(a_0, a_1, \dots, a_n) = \sum_{i=1}^m (a_0 \phi_0(x_i) + a_1 \phi_1(x_i) + \dots + a_n \phi_n(x_i) - y_i)^2.$$

To find the a_0, \dots, a_n minimising $E_2(a_0, a_1, \dots, a_n)$, require

$$\frac{\partial E_2}{\partial a_j} = \sum_{i=1}^m 2\phi_j(x_i)(a_0 \phi_0(x_i) + \dots + a_n \phi_n(x_i) - y_i) = 0.$$

Rearranging gives for $j = 0, \dots, n$

$$\sum_{i=1}^m \phi_j(x_i) \left(\sum_{k=0}^n a_k \phi_k(x_i) \right) = \sum_{i=1}^m \phi_j(x_i) y_i,$$

which yields the system of *linear* equations

$$\sum_{k=0}^n \left(\sum_{i=1}^m \phi_j(x_i) \phi_k(x_i) \right) a_k = \sum_{i=1}^m \phi_j(x_i) y_i.$$

Setting $S_{jk} = \sum_{i=1}^m \phi_j(x_i) \phi_k(x_i)$ and $r_j = \sum_{i=1}^m \phi_j(x_i) y_i$ gives $Sa = r$.

Alternatively, take averages

$$S_{jk} = \frac{1}{m} \sum_{i=1}^m \phi_j(x_i) \phi_k(x_i), \quad r_j = \frac{1}{m} \sum_{i=1}^m \phi_j(x_i) y_i.$$

For polynomial approximants $\phi_j(x) = x^j$, we then obtain

$$S_{jk} = \overline{X^j X^k} = \overline{X^{j+k}}, \quad r_j = \overline{X^j Y}.$$

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Polynomial least squares approximation

Example Fit a quadratic function to data

x_i	0.0	0.2	0.3	0.7	1.0
y_i	0.39	0.56	0.64	0.89	0.99

Compute

						sum	av
x_i	0.0	0.2	0.3	0.7	1.0	2.2	0.44
y_i	0.39	0.56	0.64	0.89	0.99	3.47	0.694
x_i^2	0.00	0.04	0.09	0.49	1.00	1.62	0.324
x_i^3	0.000	0.008	0.027	0.343	1.000	1.378	0.2756
x_i^4	0.0000	0.0016	0.0081	0.2401	1.0000	1.2498	0.24996
$x_i y_i$	0.000	0.1120	0.192	0.623	0.990	1.917	0.3834
$x_i^2 y_i$	0.0000	0.0224	0.0576	0.4361	0.9900	1.5061	0.30122

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Polynomial least squares approximation

Example Fit a quadratic function to data

x_i	0.0	0.2	0.3	0.7	1.0
y_i	0.39	0.56	0.64	0.89	0.99

Found

$$\bar{1} = 1; \quad \bar{X} = 0.44; \quad \bar{X^2} = 0.324; \quad \bar{X^3} = 0.2756; \quad \bar{X^4} = 0.24996$$

$$\bar{Y} = 0.694; \quad \overline{XY} = 0.3834; \quad \overline{X^2Y} = 0.30122;$$

Solve equations $Sa = r$ where

$$S = \begin{pmatrix} \bar{1} & \bar{X} & \bar{X^2} \\ \bar{X} & \bar{X^2} & \bar{X^3} \\ \bar{X^2} & \bar{X^3} & \bar{X^4} \end{pmatrix} = \begin{pmatrix} 1.0 & 0.44 & 0.324 \\ 0.44 & 0.324 & 0.2756 \\ 0.324 & 0.2756 & 0.24996 \end{pmatrix}; \quad r = \begin{pmatrix} \bar{Y} \\ \overline{XY} \\ \overline{X^2Y} \end{pmatrix} = \begin{pmatrix} 0.694 \\ 0.3834 \\ 0.30122 \end{pmatrix}.$$

Find $a = (0.3867, 0.9576, -0.3520)$, yielding approximation

$$g(x) = a_0 + a_1x + a_2x^2 = 0.3867 + 0.9576x - 0.3520x^2$$

Note $g(0.2) = 0.5641 \dots$, correct to precision of data.

Estimate $g(0.5) = 0.7775 = 0.78$ (2dp; precision of data).

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Polynomial least squares in Matlab

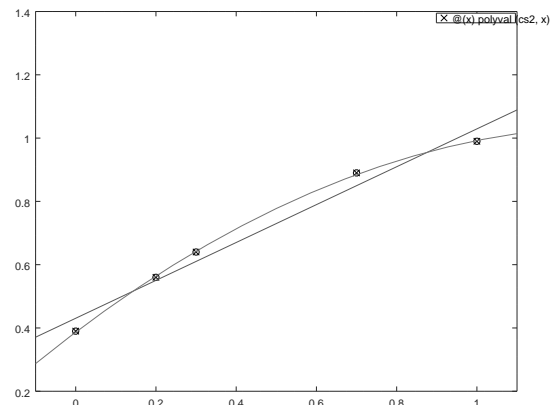
Matlab polyfit The command `polyfit(xs,ys,d)` computes the coefficients of the least-squares polynomial approximation to data `xs, ys` of degree `d`.

Example Fit a quadratic polynomial to data using Matlab.

x_i	0.0	0.2	0.3	0.7	1.0
y_i	0.39	0.56	0.64	0.89	0.99

Estimate the value of y when $x = 0.2$.

```
xs=[0.0,0.2,0.3,0.7,1.0]
ys=[0.39,0.56,0.64,0.89,0.99]
cs=polyfit(xs,ys,2)
p=@(x) polyval(cs,x)
p(0.2)
ans = 0.56414
```



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Nonlinear regression (non-examinable)

Example Fit an exponential function $g(x) = ae^{bx}$ to data

x_i	0.0	0.2	0.3	0.7	1.0
y_i	0.39	0.56	0.64	0.89	0.99

Least-squares error

$$E = \sum_{i=0}^4 (ae^{bx_i} - y_i)^2.$$

Differentiate with respect to a, b ;

$$\frac{\partial E}{\partial a} = \sum_{i=0}^4 e^{bx_i} (ae^{bx_i} - y_i) = 0; \quad \frac{\partial E}{\partial b} = \sum_{i=0}^4 ax_i e^{bx_i} (ae^{bx_i} - y_i) = 0.$$

Solve system of *nonlinear* equations to obtain $a = 0.4718$, $b = 0.7879$ (4 dp).

Note: By taking logarithms, can consider the *linear least-squares* problem with error

$$E_l = \sum_{i=0}^4 (\log(a_l) + b_l x_i - \log(y_i))^2.$$

we obtain $a_l = 0.4447$, $b_l = 0.8896$ (4 dp)

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Optimality conditions

Basis functions Given functions $\phi_0, \phi_1, \dots, \phi_n$, write $g = \sum_{j=0}^n a_j \phi_j$.

Optimality condition Minimise over a_0, a_1, \dots, a_n the weighted square error

$$\int_a^b w(x) (g(x) - f(x))^2 dx = \int_a^b w(x) (a_0 \phi_0(x) + a_1 \phi_1(x) + \dots + a_n \phi_n(x) - f(x))^2 dx$$

Differentiate with respect to a_j :

$$\int_a^b w(x) (2\phi_j(x)) (a_0 \phi_0(x) + a_1 \phi_1(x) + \dots + a_n \phi_n(x) - f(x)) dx = 0$$

So for each $j = 0, \dots, n$,

$$\sum_{k=0}^n a_k \int_a^b w(x) \phi_j(x) \phi_k(x) dx = \int_a^b w(x) f(x) \phi_j(x) dx.$$

This is a linear equation $Sa = r$ where

$$S_{jk} = \int_a^b w(x) \phi_j(x) \phi_k(x) dx; \quad r_j = \int_a^b w(x) f(x) \phi_j(x) dx.$$

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Continuous least squares

Example Compute the quadratic polynomial best approximating $f(x) = \frac{1}{x+2}$ over $[-1, +1]$.

Write $p(x) = a_0 + a_1 x + a_2 x^2$. Then $\sum_{k=0}^2 S_{jk} a_k = r_j$ for $j = 0, 1, 2$, where

$$S_{jk} = \int_{-1}^{+1} x^{j+k} dx; \quad r_j = \int_{-1}^{+1} x^j / (x+2) dx.$$

Using $\int_{-1}^{+1} x^{j+k} dx = \frac{1+(-1)^{j+k}}{j+k+1}$, these equations simplify to:

$$\begin{aligned} 2a_0 + \frac{2}{3}a_2 &= \log 3 = 1.0986; \\ \frac{2}{3}a_1 &= 2 - 2\log 3 = -0.19722; \\ \frac{2}{3}a_0 + \frac{2}{5}a_2 &= 4\log 3 - 4 = 0.39445. \end{aligned}$$

Solving gives coefficients (to 5dp)

$$a_0 = 0.49635; \quad a_1 = -0.29584; \quad a_2 = 0.15888.$$

The approximant is

$$p(x) = 0.49635 - 0.29584x + 0.15888x^2.$$

Compute approximations

$$p(0.5) = 0.38815 = 0.39 \text{ (2dp)}; \quad f(0.5) = \frac{2}{5} = 0.40000.$$

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Orthogonal bases

Orthogonal bases We say the basis functions $\phi_0, \phi_1, \dots, \phi_n$ are *orthogonal* if

$$\int_a^b w(x) \phi_j(x) \phi_k(x) dx = 0 \text{ for } j \neq k.$$

Then for each $j = 0, \dots, n$:

$$\sum_{k=0}^n c_k \int_a^b w(x) \phi_j(x) \phi_k(x) dx = c_j \int_a^b w(x) \phi_j(x) \phi_j(x) dx,$$

since all terms vanish unless $k = j$.

The optimality conditions for $\sum_{k=0}^n c_k \phi_k(x)$ simplify to

$$c_j = \frac{\int_a^b w(x) f(x) \phi_j(x) dx}{\int_a^b w(x) \phi_j(x)^2 dx}.$$

The denominator is independent of f , so can be pre-computed. Then

$$c_j = \frac{1}{\alpha_j} \int_a^b w(x) f(x) \phi_j(x) dx \quad \text{where } \alpha_j := \int_a^b w(x) (\phi_j(x))^2 dx > 0.$$

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Generating orthogonal bases

Generating orthogonal bases An orthogonal basis of polynomials can be generated by

$$\phi_0(x) = 1, \quad \phi_1(x) = x - B_1,$$

$$\phi_k(x) = (x - B_k) \phi_{k-1}(x) - C_k \phi_{k-2}(x)$$

where

$$B_k = \frac{\int_a^b w(x) x (\phi_{k-1}(x))^2 dx}{\int_a^b w(x) (\phi_{k-1}(x))^2 dx}; \quad C_k = \frac{\int_a^b w(x) x \phi_{k-1}(x) \phi_{k-2}(x) dx}{\int_a^b w(x) (\phi_{k-2}(x))^2 dx}.$$

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Orthogonal bases (Non-examinable)

Write $\phi_k(x) = x \phi_{k-1}(x) - \sum_{i=0}^{k-1} a_i \phi_i(x)$. Take inner product with ϕ_j for $j < k$. By orthogonality

$$\begin{aligned} 0 &= \int_a^b w(x) \phi_j(x) \phi_k(x) dx \\ &= \int_a^b w(x) \phi_j(x) (x \phi_{k-1}(x) - \sum_{i=0}^{k-1} a_i \phi_i(x)) dx \\ &= \int_a^b w(x) x \phi_j(x) \phi_{k-1}(x) dx - \sum_{i=0}^{k-1} a_i \int_a^b w(x) \phi_i(x) \phi_j(x) dx \\ &= \int_a^b w(x) x \phi_j(x) \phi_{k-1}(x) dx - a_j \int_a^b w(x) \phi_j(x)^2 dx \end{aligned}$$

Since $x \phi_j(x)$ is a polynomial of degree $j + 1$,

$$\int_a^b w(x) x \phi_j(x) \phi_{k-1}(x) dx = 0 \text{ if } j + 1 < k - 1.$$

Hence

$$a_j = \begin{cases} \frac{\int_a^b w(x) x \phi_j(x) \phi_{k-1}(x) dx}{\int_a^b w(x) \phi_j(x)^2 dx} & \text{for } j = k - 2, k - 1; \\ 0 & \text{for } j = 0, \dots, k - 3. \end{cases}$$

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Legendre polynomials

Legendre polynomials The *monic Legendre polynomials* P_k form an orthogonal basis over $[-1, +1]$ with respect to the weight function $w(x) \equiv 1$.

$$P_0(x) = 1.$$

$$B_1 = \frac{\int_{-1}^{+1} x(P_0(x))^2 dx}{\int_{-1}^{+1} (P_0(x))^2 dx} = \frac{\int_{-1}^{+1} x \cdot 1^2 dx}{\int_{-1}^{+1} 1^2 dx} = 0;$$

$$P_1(x) = x - B_1 = x - 0 = x.$$

$$B_2 = \frac{\int_{-1}^{+1} x(P_1(x))^2 dx}{\int_{-1}^{+1} (P_1(x))^2 dx} = \frac{\int_{-1}^{+1} x \cdot x^2 dx}{\int_{-1}^{+1} x^2 dx} = 0;$$

$$C_2 = \frac{\int_{-1}^{+1} xP_1(x)P_0(x) dx}{\int_{-1}^{+1} (P_0(x))^2 dx} = \frac{\int_{-1}^{+1} x \cdot x \cdot 1 dx}{\int_{-1}^{+1} 1^2 dx} = \frac{2/3}{2} = \frac{1}{3};$$

$$P_2(x) = (x - B_2)P_1(x) - C_2P_0(x) = (x - 0)x - \frac{1}{3} = x^2 - \frac{1}{3}.$$

$$B_3 = \frac{\int_{-1}^{+1} x(P_2(x))^2 dx}{\int_{-1}^{+1} (P_2(x))^2 dx} = \frac{\int_{-1}^{+1} x \cdot (x^2 - \frac{1}{3})^2 dx}{\int_{-1}^{+1} (x^2 - \frac{1}{3})^2 dx} = 0;$$

$$C_3 = \frac{\int_{-1}^{+1} xP_2(x)P_1(x) dx}{\int_{-1}^{+1} (P_1(x))^2 dx} = \frac{\int_{-1}^{+1} x \cdot (x^2 - \frac{1}{3}) \cdot x dx}{\int_{-1}^{+1} x^2 dx} = \frac{\int_{-1}^{+1} x^4 - \frac{1}{3}x^2 dx}{\int_{-1}^{+1} x^2 dx} = \frac{2/5 - 2/9}{2/3} = \frac{4}{15};$$

$$P_3(x) = (x - B_3)P_2(x) - C_3P_1(x) = (x - 0)(x^2 - \frac{1}{3}) - \frac{4}{15}x = x^3 - \frac{3}{5}x.$$

$$P_4(x) = (x - B_4)P_3(x) - C_4P_2(x) = (x - 0)(x^3 - \frac{3}{5}x) - \frac{9}{35}(x^2 - \frac{1}{3}) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$$

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Legendre polynomials

Legendre polynomials Usually easier to use *normalised* polynomials with

$$P_k(1) = 1 \text{ for all } k.$$

Recurrence relation

$$\begin{aligned} P_k(x) &= ((2k-1)xP_{k-1}(x) - (k-1)P_{k-2}(x))/k \\ &= (2 - \frac{1}{k})xP_{k-1}(x) - (1 - \frac{1}{k})P_{k-2}(x). \end{aligned}$$

Orthogonality

$$\int_{-1}^1 P_i(x) P_j(x) dx = 0, \quad i \neq j.$$

Norms

$$\|P_k\|^2 := \int_{-1}^{+1} P_k^2(x) dx = \frac{2}{2k+1} = \frac{1}{k+1/2}.$$

Coefficients

$$c_k = (k + \frac{1}{2}) \int_{-1}^{+1} P_k(x) f(x) dx.$$

Explicit formulae

$$\begin{aligned} P_0(x) &= 1; \quad P_1(x) = x; \quad P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}; \\ P_3(x) &= \frac{5}{2}x^3 - \frac{3}{2}x; \quad P_4(x) = \frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}. \end{aligned}$$

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Legendre polynomials

Example Compute the quartic least-squares polynomial approximation to $f(x) = 1/(x+2)$ on $[-1, 1]$.

Write $p(x) = \sum_{k=0}^4 c_k P_k(x)$ where by orthogonality and normalisation

$$c_k = \frac{\int_{-1}^{+1} f(x) P_k(x) dx}{\int_{-1}^{+1} P_k(x)^2 dx} = \frac{\int_{-1}^{+1} f(x) P_k(x) dx}{2/(2k+1)} = (k + \frac{1}{2}) \int_{-1}^{+1} f(x) P_k(x) dx.$$

Compute integrals analytically or numerically.

$$c_0 = \frac{1}{2} \int_{-1}^{+1} \frac{1}{x+2} dx = \frac{1}{2} \log 3 = \frac{1}{2} \times 1.0986 = 0.5493$$

$$c_1 = \frac{3}{2} \int_{-1}^{+1} \frac{1}{x+2} x dx = \frac{3}{2} (2 - 2 \log 3) = \frac{3}{2} \times (-0.1972) = -0.2958$$

$$c_2 = \frac{5}{2} \int_{-1}^{+1} \frac{1}{x+2} (\frac{3}{2}x^2 - \frac{1}{2}) dx = \frac{5}{2} (\frac{11}{2} \log 3 - 6) = \frac{5}{2} \times 0.0424 = 0.1059$$

$$c_3 = \frac{7}{2} \int_{-1}^{+1} \frac{1}{x+2} (\frac{5}{2}x^3 - \frac{3}{2}x) dx = \frac{7}{2} \times (-0.0341) = -0.0341$$

$$c_4 = \frac{9}{2} \int_{-1}^{+1} \frac{1}{x+2} (\frac{35}{8}x^4 - \frac{15}{4}x^2 + \frac{3}{8}) dx = \frac{9}{2} \times 0.00232 = 0.0104$$

Approximating polynomial

$$g(x) = 0.549P_0(x) - 0.296P_1(x) + 0.106P_2(x) - 0.034P_3(x) + 0.010P_4(x)$$

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Evaluating Legendre polynomials

Recurrence relation It is more efficient and accurate to use the recurrence relation to evaluate Legendre polynomials, than to evaluate them directly!

$$P_0(x) = 1;$$

$$P_1(x) = x;$$

$$P_2(x) = \frac{3}{2}xP_1(x) - \frac{1}{2}P_0(x);$$

$$P_3(x) = \frac{5}{3}xP_2(x) - \frac{2}{3}P_1(x);$$

$$P_4(x) = \frac{7}{4}xP_3(x) - \frac{3}{4}P_2(x);$$

$$P_5(x) = \frac{9}{5}xP_4(x) - \frac{4}{5}P_3(x).$$

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Evaluating Legendre polynomials

Example Evaluate at $x = 0.6$ the function

$$g(x) = 0.549P_0(x) - 0.296P_1(x) + 0.106P_2(x) - 0.034P_3(x) + 0.010P_4(x).$$

$$P_0(0.6) = 1.000;$$

$$P_1(0.6) = 0.600;$$

$$P_2(0.6) = \frac{3}{2} \times 0.6 \times P_1(0.6) - \frac{1}{2} \times P_0(0.6) = \frac{3}{2} \times 0.6 \times 0.600 - \frac{1}{2} \times 1.000 = 0.040;$$

$$P_3(0.6) = \frac{5}{3} \times 0.6 \times P_2(0.6) - \frac{2}{3} \times P_1(0.6) = \frac{5}{3} \times 0.6 \times 0.040 - \frac{2}{3} \times 0.600 = -0.360;$$

$$P_4(0.6) = \frac{7}{4} \times 0.6 \times P_3(0.6) - \frac{3}{4} \times P_2(0.6) = \frac{7}{4} \times 0.6 \times (-0.360) - \frac{3}{4} \times 0.040 = -0.408;$$

$$\begin{aligned} g(0.6) &= 0.549 \times 1.0 - 0.296 \times 0.6 + 0.106 \times 0.04 - 0.034 \times (-0.36) + 0.010 \times (-0.408) \\ &= 0.5490 - 0.1776 + 0.0042 + 0.0122 - 0.0041 = 0.384 \text{ (3dp)} \end{aligned}$$

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Legendre polynomials

Evaluation in Matlab Compute array of function values recursively, with $P_{xs}(k+1)$ storing $P_k(x)$:

```
function Pxs = legendre(x,n)
    Pxs(0+1)=1;
    Pxs(1+1)=x;
    for k=2:n,
        Pxs(k+1)=( (2*k-1)*x.*Pxs(k-1+1)-(k-1)*Pxs(k-2+1) )/k;
    end;
```

Compute coefficients using integral of vector-valued function:

```
alphas=1./((0:n)+0.5);
f_times_P=@(x)f(x)*legendre(x,n);
cs=integral(f_times_P,-1,+1,'ArrayValued',true)./alphas;
```

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Chebyshev polynomials

Chebyshev functions The Chebyshev functions T_j form an orthogonal basis of polynomials on $[-1, +1]$ with respect to the weight $w(x) = 1/\sqrt{1-x^2}$.

Cosine formula $T_k(x) = \cos(k \arccos(x))$.

Recurrence formula $T_0(x) = 1$, $T_1(x) = x$, $T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$.

Orthogonality $\int_{-1}^{+1} T_i(x)T_j(x)/\sqrt{1-x^2} dx = 0$ for $i \neq j$:

$$\int_{-1}^{+1} w(x)T_k(x)^2 dx = \pi/2 \text{ for } k \geq 1,$$

$$\int_{-1}^{+1} w(x)T_0(x)^2 dx = \pi.$$

Coefficients

$$c_0 = \frac{1}{\pi} \int_{-1}^{+1} w(x) f(x) dx = \frac{1}{\pi} \int_0^\pi f(\cos \theta) d\theta$$

$$\text{For } k \geq 1, c_k = \frac{2}{\pi} \int_{-1}^{+1} w(x) T_k(x) f(x) dx = \frac{2}{\pi} \int_0^\pi \cos(k\theta) f(\cos \theta) d\theta$$

The integral in θ is usually more accurate since $\lim_{x \rightarrow \pm 1} w(x) = \infty$.

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Chebyshev polynomials

Check orthogonality

$$\begin{aligned}\int_{-1}^{+1} \frac{T_m(x)T_n(x)}{\sqrt{1-x^2}} dx &= \int_{-1}^{+1} \frac{\cos(m \arccos(x)) \cos(n \arccos(x))}{\sqrt{1-x^2}} dx \\&= \int_{\pi}^0 \frac{\cos(m\theta) \cos(n\theta)}{\sqrt{1-\cos^2(\theta)}} (-\sin \theta) d\theta \quad [x = \cos \theta] \\&= \int_0^{\pi} -\frac{\cos(m\theta) \cos(n\theta)}{\sqrt{\sin^2(\theta)}} (-\sin \theta) d\theta \\&= \int_0^{\pi} \cos(m\theta) \cos(n\theta) d\theta \\&= \int_0^{\pi} \frac{1}{2} (\cos((m+n)\theta) + \cos((n-m)\theta)) d\theta \\&= \left[\frac{1}{2(m+n)} \sin((m+n)\theta) + \frac{1}{2(n-m)} \sin((n-m)\theta) \right]_0^{\pi} \quad (m \neq n) \\&= \frac{1}{2(m+n)} \sin((m+n)\pi) + \frac{1}{2(n-m)} \sin((n-m)\pi) \\&= 0 \quad (m \neq n)\end{aligned}$$

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Chebyshev polynomials

Explicit formulae The Chebyshev polynomials up to degree 6 are

$$\begin{aligned}T_0(x) &= 1; \quad T_1(x) = x; \quad T_2(x) = 2x^2 - 1 \\T_3(x) &= 4x^3 - 3x; \quad T_4(x) = 8x^4 - 8x^2 + 1 \\T_5(x) &= 16x^5 - 20x^3 + 5x; \quad T_6(x) = 32x^6 - 48x^4 + 18x^2 - 1\end{aligned}$$

Recurrence formula It is more efficient and accurate to evaluate the Chebyshev polynomials by $T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$.

$$\begin{aligned}T_0(0.6) &= 1 = 1.0000; \\T_1(0.6) &= 0.6 = 0.6000; \\T_2(0.6) &= 2 \times 0.6 \times T_1(0.6) - T_0(0.6) = 2 \times 0.6 \times (0.6000) - 1.0000 = -0.2800; \\T_3(0.6) &= 2 \times 0.6 \times T_2(0.6) - T_1(0.6) = 2 \times 0.6 \times (-0.2800) - 0.6000 = -0.9360; \\T_4(0.6) &= 2 \times 0.6 \times T_3(0.6) - T_2(0.6) = 2 \times 0.6 \times (-0.9360) + 0.2800 = -0.8432; \\T_5(0.6) &= 2 \times 0.6 \times T_4(0.6) - T_3(0.6) = 2 \times 0.6 \times (-0.8432) + 0.9360 = -0.0758; \\T_6(0.6) &= 2 \times 0.6 \times T_5(0.6) - T_4(0.6) = 2 \times 0.6 \times (-0.0758) + 0.8432 = 0.7522.\end{aligned}$$

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Chebyshev polynomials

Example Compute the quartic polynomial approximating $f(x) = 1/(x+2)$ over $[-1, +1]$ with respect to the weight $1/\sqrt{1-x^2}$.

Numerically find (to 4dp)

$$c_0 = \frac{1}{\pi} \int_0^\pi f(\cos(\theta)) d\theta = \frac{1}{\pi} \int_0^\pi \frac{1}{\cos(\theta)+2} d\theta = 0.5774$$

$$c_1 = \frac{2}{\pi} \int_0^\pi f(\cos(\theta)) \cos(\theta) d\theta = \frac{2}{\pi} \int_0^\pi \frac{\cos(\theta)}{\cos(\theta)+2} d\theta = -0.3094$$

$$c_2 = \frac{2}{\pi} \int_0^\pi f(\cos(\theta)) \cos(2\theta) d\theta = \frac{2}{\pi} \int_0^\pi \frac{\cos(2\theta)}{\cos(\theta)+2} d\theta = 0.0829$$

$$c_3 = \frac{2}{\pi} \int_0^\pi f(\cos(\theta)) \cos(3\theta) d\theta = \frac{2}{\pi} \int_0^\pi \frac{\cos(3\theta)}{\cos(\theta)+2} d\theta = -0.0222$$

$$c_4 = \frac{2}{\pi} \int_0^\pi f(\cos(\theta)) \cos(4\theta) d\theta = \frac{2}{\pi} \int_0^\pi \frac{\cos(4\theta)}{\cos(\theta)+2} d\theta = 0.0060$$

Approximating polynomial

$$p(x) = 0.5774T_0(x) - 0.3094T_1(x) + 0.0829T_2(x) - 0.0222T_3(x) + 0.0060T_4(x).$$

Check to 4dp: $p(0.2) = 0.4559$, $f(0.2) = 0.4545$. Relative error 0.3%.

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Errors in orthogonal bases

Least-squares error The square error in approximating f by $g_n(x) = \sum_{k=0}^n c_k \phi_k(x)$ is

$$E_2 = \int_a^b w(x)(f(x) - g_n(x))^2 dx = \int_a^b w(x)f(x)^2 dx - \sum_{k=0}^n \alpha_k c_k^2,$$

where $\alpha_k = \int_a^b w(x)\phi_k(x)^2 dx$.

In particular, the difference between the error of g_{n-1} and g_n is $\alpha_n c_n^2$.

Infinite series If $f(x) = \sum_{k=0}^\infty c_k \phi_k(x)$, then

$$\int_a^b w(x)(f(x) - g_n(x))^2 dx = \sum_{k=n+1}^\infty \alpha_k c_k^2$$

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Uniform Approximation (Non-examinable)

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Uniform function approximation

Uniform function approximation Given $f : [a, b] \rightarrow \mathbb{R}$, find a function g approximating f minimising error

$$E = \sup_{x \in [a, b]} |g(x) - f(x)|.$$

Remez Algorithm Algorithm for constructing polynomial of best uniform approximation.

Uniform spline/Fourier approximation Similar results hold for uniform approximation by splines and Fourier series

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Fourier series

Fourier approximation Approximate f on $[-\pi, \pi]$ in the least-squares error by a function of the form

$$s_n(x) = \frac{a_0}{2} + \sum_{k=1}^n a_k \cos(kx) + b_k \sin(kx)$$

Orthogonality

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \cos(mx) \sin(nx) dx = 0 \text{ for all } m, n \in \mathbb{N}.$$

$$\frac{1}{\pi} \int_{-\pi}^{\pi} \cos(mx) \cos(nx) dx = \frac{1}{\pi} \int_{-\pi}^{\pi} \sin(mx) \sin(nx) dx = 0 \text{ for } m \neq n.$$

Coefficients

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx) dx; \quad b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx) dx.$$

Fourier series If f is continuous, then

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos(kx) + b_k \sin(kx)$$

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Fourier series**Orthogonality**

$$\begin{aligned} \int_{-\pi}^{\pi} \cos(mx) \cos(nx) dx &= \int_{-\pi}^{\pi} \frac{1}{2} \cos((m-n)x) + \frac{1}{2} \cos((m+n)x) dx \\ &\stackrel{m \neq n}{=} \left[\frac{\sin((m-n)x)}{2(m-n)} + \frac{\sin((m+n)x)}{2(m+n)} \right]_{-\pi}^{\pi} \\ &= \frac{\sin((m-n)\pi) - \sin(-(m-n)\pi)}{2(m-n)} + \frac{\sin((m+n)\pi) - \sin(-(m+n)\pi)}{2(m+n)} \\ &= \frac{0-0}{2(m-n)} + \frac{0-0}{2(m+n)} = 0 \end{aligned}$$

For the case $m = n \neq 0$,

$$\begin{aligned} \int_{-\pi}^{\pi} \cos(nx) \cos(nx) dx &= \int_{-\pi}^{\pi} \cos^2(nx) dx = \int_{-\pi}^{\pi} \frac{1}{2} - \frac{1}{2} \cos(2nx) dx \\ &= \left[\frac{x}{2} + \frac{\sin(2nx)}{2 \times 2n} \right]_{-\pi}^{\pi} = \frac{\pi - (-\pi)}{2} + \frac{\sin(2n\pi) - \sin(-2n\pi)}{4n} \\ &= \frac{2\pi}{2} + \frac{0-0}{4n} = \pi \end{aligned}$$

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Fourier series

Approximation error The error in approximating $f(x)$ by $s_n(x)$ is

$$\int_{-\pi}^{\pi} (f(x) - s_n(x))^2 dx = \int_{-\pi}^{\pi} f(x)^2 dx - \pi \left(\frac{a_0^2}{2} + \sum_{k=1}^n (a_k^2 + b_k^2) \right) = \pi \sum_{k=n+1}^{\infty} (a_k^2 + b_k^2).$$

Square integral The square integral of f is

$$\int_{-\pi}^{+\pi} f(x)^2 dx = \pi \left(\frac{a_0^2}{2} + \sum_{k=1}^{\infty} (a_k^2 + b_k^2) \right).$$

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Fourier series

Even and odd functions A function is *even* if $f(-x) = f(x)$ for all x , and *odd* if $f(-x) = -f(x)$.

If f is an even function, then for any k ,

$$a_k := \frac{1}{\pi} \int_{-\pi}^{+\pi} f(x) \cos(kx) dx = \frac{2}{\pi} \int_0^{\pi} f(x) \cos(kx) dx;$$

$$b_k := \frac{1}{\pi} \int_{-\pi}^{+\pi} f(x) \sin(kx) dx = 0.$$

If f is an odd function, then for any k ,

$$a_k = 0; \quad b_k = \frac{2}{\pi} \int_0^{\pi} f(x) \sin(kx) dx.$$

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Fourier series

Example Approximate $f(x) = \sin(2x)/(3 + \sin(x) + 2 \cos(x))$ by a Fourier sum with $n = 3$.

$$a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) dx = 0.16000$$

$$a_1 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(x) dx = 0.14400$$

$$a_2 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(2x) dx = 0.01920$$

$$a_3 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(3x) dx = 0.09344$$

$$b_1 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(x) dx = -0.19200$$

$$b_2 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(2x) dx = 0.50560$$

$$b_3 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(3x) dx = -0.20608$$

So Fourier approximation is

$$f(x) \approx s_3(x) = 0.160 - 0.144 \cos(x) - 0.192 \sin(x) + 0.019 \cos(2x) \\ + 0.506 \sin(2x) + 0.093 \cos(3x) - 0.206 \sin(3x).$$

Notice that b_2 is the largest coefficient, due to the dominating effect of the $\sin(2x)$ factor.

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Fourier series

Example Approximate $f(x) = x$ on $[-\pi, +\pi]$ by a Fourier series.

Since f is an odd function, for any k ,

$$a_k = 0; \quad b_k = \frac{2}{\pi} \int_0^{\pi} f(x) \sin(kx) dx$$

Then since

$$\begin{aligned} \int x \sin(kx) dx &= -x \cos(kx)/k + \int \cos(kx)/k dx \\ &= \sin(kx)/k^2 - x \cos(kx)/k \end{aligned}$$

we have

$$\begin{aligned} b_k &= \frac{1}{\pi} \int_{-\pi}^{+\pi} f(x) \sin(kx) dx = \frac{2}{\pi} \int_0^{\pi} f(x) \sin(kx) dx \\ &= \frac{2}{\pi} [\sin(kx)/k^2 - x \cos(kx)/k]_0^{\pi} = \frac{2}{\pi} (-\pi \cos(k\pi)/k) = (-1)^{k-1} 2/k \end{aligned}$$

The Fourier series is

$$f(x) = \sum_{k=1}^{\infty} (-1)^{k-1} (2/k) \sin(kx).$$

with finite approximations

$$\begin{aligned} f(x) &\approx s_n(x) = \sum_{k=1}^n (-1)^{k-1} (2/k) \sin(kx). \\ s_6(x) &= 2 \sin(x) - \sin(2x) + \frac{2}{3} \sin(3x) - \frac{1}{2} \sin(4x) + \frac{2}{5} \sin(5x) - \frac{1}{3} \sin(6x). \end{aligned}$$

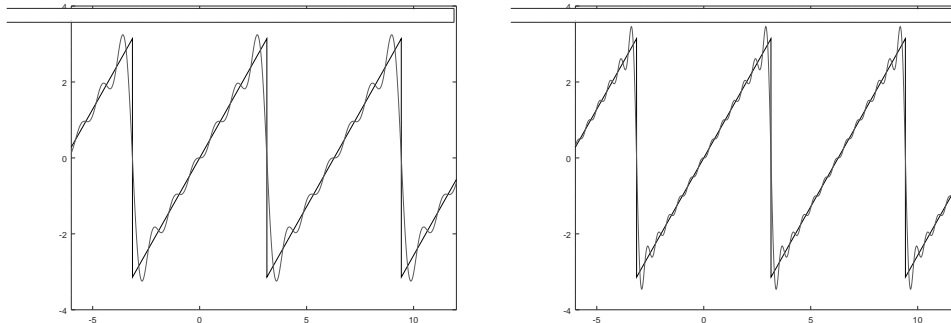
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Gibbs phenomenon

Sawtooth wave Extending $f(x) = x$ on $[-\pi, \pi]$ to a 2π -periodic function give the *sawtooth wave*
 $f(x) = x - 2\pi \lfloor x/2\pi \rfloor$,

where $\lfloor r \rfloor$ denotes the nearest integer to r .

The Fourier approximations for $n = 6$ and $n = 12$ are given below:



There is a small overshoot (around 9%) near the discontinuity!

This overshoot is known as the *Gibbs phenomenon*, and *always* occurs in the Fourier expansion of a function near discontinuities.

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Convergence of Fourier series

Theorem Let f be a piecewise-continuous 2π -periodic function, which is *square-integrable* in the sense that $\int_{-\pi}^{+\pi} f(x)^2 dx < \infty$.

Then the Fourier approximations s_n converge *pointwise* to f , and in the *root-mean-square error*, but not *uniformly* near discontinuity points of f .

If f is continuous, then the Fourier approximations converge uniformly.

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Rescaling

Periodic functions f is periodic with period T if $f(t + T) = f(t)$ for all t .

Fourier series If f is T -periodic, then

$$f(t) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos\left(\frac{2\pi kt}{T}\right) + b_k \sin\left(\frac{2\pi kt}{T}\right),$$

Coefficients

$$a_k = \frac{2}{T} \int_0^T f(t) \cos\left(\frac{2\pi kt}{T}\right) dt; \quad b_k = \frac{2}{T} \int_0^T f(t) \sin\left(\frac{2\pi kt}{T}\right) dt.$$

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Discrete Fourier transform

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Discrete Fourier transform

Discrete Fourier series Approximate data (x_i, y_i) where $x_i = \pi i/m$ for $i = -m, \dots, m-1$ by a function of the form

$$s_n(x) = \frac{a_0}{2} + \sum_{k=1}^n a_k \cos(kx) + b_k \sin(kx)$$

Orthogonality

$$\frac{1}{m} \sum_{i=-m}^{m-1} \cos(n_1 x_i) \sin(n_2 x_i) = \frac{1}{m} \sum_{i=-m}^{m-1} \cos(n_1 \pi i/m) \sin(n_2 \pi i/m) = 0 \text{ for all } n_1, n_2 \in \mathbb{N}.$$

$$\frac{1}{m} \sum_{i=-m}^{m-1} \cos(n_1 \pi i/m) \cos(n_2 \pi i/m) = \frac{1}{m} \sum_{i=-m}^{m-1} \sin(n_1 \pi i/m) \sin(n_2 \pi i/m) = 0 \text{ for } n_1 \neq n_2.$$

Coefficients

$$a_k = \frac{1}{m} \sum_{i=-m}^{m-1} y_i \cos(kx_i); \quad b_k = \frac{1}{m} \sum_{i=-m}^{m-1} y_i \sin(kx_i).$$

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Discrete Fourier transform

Trigonometric values for $m = 4, 6, 8$

x_i	0	$\pi/8$	$\pi/6$	$\pi/4$	$\pi/3$	$3\pi/8$	$\pi/2$
$\cos(x_i)$	1	$\frac{1}{2}\sqrt{2+\sqrt{2}}$	$\sqrt{3}/2$	$1/\sqrt{2}$	$1/2$	$\frac{1}{2}\sqrt{2-\sqrt{2}}$	0
$\cos(x_i)$	1.00000	0.92388	0.86603	0.70711	0.50000	0.38268	0.00000
$\sin(x_i)$	0	$\frac{1}{2}\sqrt{2-\sqrt{2}}$	$1/2$	$1/\sqrt{2}$	$\sqrt{3}/2$	$\frac{1}{2}\sqrt{2+\sqrt{2}}$	1
$\sin(x_i)$	0.00000	0.38268	0.50000	0.70711	0.86603	0.92388	1.00000

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Discrete Fourier transform

Example Approximate data $y_i = f(x_i)$ with $m = 4$ where $f(x) = e^{-x^2/4}$ by $s_2(x) = \frac{a_0}{2} + \sum_{k=1}^2 a_k \cos(kx) + b_k \sin(kx)$.

i	-4	-3	-2	-1	0	$+1$	$+2$	$+3$	$+4$
x_i	$-\pi$	$-3\pi/4$	$-\pi/2$	$-\pi/4$	0	$\pi/4$	$\pi/2$	$3\pi/4$	π
y_i	0.085	0.250	0.540	0.857	1.000	0.857	0.540	0.250	0.085

Compute values of $y_i \cos(kx_i)$ and $y_i \sin(kx_i)$:

x_i	$-\pi$	$-3\pi/4$	$-\pi/2$	$-\pi/4$	0	$\pi/4$	$\pi/2$	$3\pi/4$	sum
y_i	0.085	0.250	0.540	0.857	1.000	0.857	0.540	0.250	4.379
$y_i \cos(x_i)$	-0.085	-0.177	0.000	0.606	1.000	0.606	0.000	-0.177	1.773
$y_i \cos(2x_i)$	0.085	0.000	-0.540	0.000	1.000	0.000	-0.540	0.000	0.005
$y_i \sin(x_i)$	0.000	-0.177	-0.540	-0.606	0.000	0.606	0.540	0.177	0.000
$y_i \sin(2x_i)$	0.000	0.250	-0.000	-0.857	0.000	0.857	0.000	-0.250	0.000

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Discrete Fourier transform

Example Approximate data $y_i = f(x_i)$ with $m = 4$ by Fourier approximant s_2 .

i	-4	-3	-2	-1	0	$+1$	$+2$	$+3$	$+4$
x_i	$-\pi$	$-3\pi/4$	$-\pi/2$	$-\pi/4$	0	$\pi/4$	$\pi/2$	$3\pi/4$	π
y_i	0.085	0.250	0.540	0.857	1.000	0.857	0.540	0.250	0.085

Compute coefficients (to 3dp):

$$a_0 = \frac{1}{4} \sum_{i=-4}^3 y_i = 1.095$$

$$a_1 = \frac{1}{4} \sum_{i=-4}^3 y_i \cos(x_i) = 0.443$$

$$a_2 = \frac{1}{4} \sum_{i=-4}^3 y_i \cos(2x_i) = 0.001$$

$$b_1 = \frac{1}{4} \sum_{i=-4}^3 y_i \sin(x_i) = 0$$

$$b_2 = \frac{1}{4} \sum_{i=-4}^3 y_i \sin(2x_i) = 0$$

So discrete Fourier transform is

$$f(x) \approx s_2(x) = 0.547 + 0.443 \cos(x) + 0.001 \cos(2x).$$

Estimate $s_2(1) = 0.786$ (3dp), exact $f(1) = 0.77880$; relative error $\approx 1\%$.

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Discrete Fourier transform

Example Approximate data (x_i, y_i) with $m = 3$ by $s_2(x)$.

i	-3	-2	-1	0	+1	+2	+3
x_i	$-\pi$	$-2\pi/3$	$-\pi/3$	0	$\pi/3$	$2\pi/3$	π
y_i	0.000	0.764	-0.276	0.000	0.178	-0.302	0.000

Compute values of $y_i \cos(kx_i)$ and $y_i \sin(kx_i)$:

x_i	$-\pi$	$-2\pi/3$	$-\pi/3$	0	$\pi/3$	$2\pi/3$	sum	coef
y_i	0.000	0.764	-0.276	0.000	0.178	-0.302	0.364	0.121
$y_i \cos(x_i)$	-0.000	-0.382	-0.138	0.000	0.089	0.151	-0.280	-0.093
$y_i \sin(x_i)$	-0.000	-0.662	0.239	0.000	0.154	-0.262	-0.530	-0.177
$y_i \cos(2x_i)$	0.000	-0.382	0.138	0.000	-0.089	0.151	-0.182	-0.061
$y_i \sin(2x_i)$	0.000	0.662	0.239	0.000	0.154	0.262	1.316	0.439

So discrete Fourier transform is

$$f(x) \approx s_2(x) = 0.061 - 0.093 \cos(x) - 0.177 \sin(x) - 0.061 \cos(2x) + 0.439 \sin(2x).$$

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Fast Fourier transform (Non-examinable)

Complexity-DFT Computing all terms of the discrete Fourier transform for n data points takes time $\Theta(n^2)$.

For many applications, the data is so big that this is too slow!

Complexity-FFT The fast Fourier transform (FFT) is an algorithm which can compute the coefficients in time $\Theta(n \log n)$

It uses the complex form $e^{i\theta} = \cos(\theta) + i \sin(\theta)$, and computes complex coefficients $c_k = a_k + ib_k$.

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