Fast spectral methods in theory & practice

$L^2(0,1)$

Consider functions on $(0,1)$.

$\langle f,g\rangle = \int_0^1 f(x)g(x)\,dx$ inner product

$\|f\|_2 = (\langle f,f\rangle)^{\frac{1}{2}}$ norm

$L^2(0,1) = \{ f(x) : \int_0^1 (f(x))^2\,dx < \infty \}$ plus all Cauchy sequences to make this a Hilbert space.

Orthogonal $0 \neq f,g$ orthogonal means $\langle f,g\rangle = 0$.

Complete $\{\varphi_k(x)\}_{k\in\mathbb{N}}$ is complete means that for all $f \in L^2$ & $\epsilon > 0$, there exists $\{\varphi_{j_1}, \dots, \varphi_{j_N}\}$ and $\{a_\ell\}_{\ell=1}^N$ such that

$$\boxed{\left\| \sum_{\ell=1}^N a_\ell \varphi_\ell(x) - f \right\|_2 < \epsilon.}$$

That is f is arbitrarily well approximable by $\{\varphi_k\}$.

Trigonometric polynomials

Consider the trigonometric polynomials $\cos(n\pi x)$ and $\sin(n\pi x)$ on $[0,1]$, $n=0,1,2$

Facts: The following three sets are complete & orthogonal

$\left\{ \cos(k\pi x) \right\}_{k=0}^{\infty}$ — $\varphi_k'(0) = \varphi_k'(1) = 0$ Neumann boundary conditions

$\left\{ \sin(k\pi x) \right\}_{k=1}^{\infty}$ — $\varphi_k(0) = \varphi_k(1) = 0$ Dirichlet boundary conditions

$\left\{ \cos(2k\pi x) \right\}_{k=0}^{\infty} \cup \left\{ \sin 2k\pi x \right\}_{k=1}^{\infty}$ — $\varphi_k(0) = \varphi_k(1)$, $\varphi_k'(0) = \varphi_k'(1)$ Periodic boundary conditions

Given a function $f \in L^2(0,1)$ and given N, how can we numerically determine $a_1, \dots, a_N$ such that

$f_N = \sum_{k=1}^{N} a_k \varphi_k(x)$ best approximates f

ie. minimize $\|f - f_N\|_2$.

Trigonometric Interpolation

Given points $0 \leq t_1 < t_2 < \cdots < t_n \leq b$

and $x_k = f(t_k) \qquad k = 1, \ldots, n$

find interpolating function

$$\varphi(t) = \sum_{\ell=1}^{n} \alpha_\ell \varphi_\ell(t) \quad \text{with} \quad \varphi(t_k) = x_k$$

This is actually a linear problem

$$\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} \varphi_1(t_1) & \cdots & \varphi_n(t_1) \\ \varphi_1(t_2) & \cdots & \varphi_n(t_2) \\ \vdots & \ddots & \vdots \\ \varphi_1(t_n) & \cdots & \varphi_n(t_n) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}$$

Discrete cosine transform

Let $c_0 = 1$, $c_\ell = \sqrt{2}$ $\ell \neq 0$ & $t_\ell = \frac{2\ell+1}{2n}$

Given $x = (x_0, \ldots, x_{n-1})$

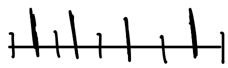
$dct(x) = y$ where $y_k = \frac{c_k}{\sqrt{n}} \sum_{\ell=0}^{n-1} x_\ell \cos(\pi k t_\ell)$

$idct(y) = x$ where $x_k = \frac{1}{\sqrt{n}} \sum_{\ell=0}^{n-1} y_\ell c_\ell \cos(\pi \ell t_k)$

Theorem $\varphi(t) = \sum_{\ell=0}^{n-1} \frac{y_\ell c_\ell}{\sqrt{n}} \cos(\ell \pi t)$ is the best approx & unique cosine interpolant of $x_k = f(t_k)$

Example

$x = (1, 2, -3, 0) \qquad t = \left(\frac{1}{8}, \frac{3}{8}, \frac{5}{8}, \frac{7}{8}\right)$



$y = \text{dct}(x) = (0, 2.00627, 1, -2.99581)$

$\alpha = \frac{y}{\sqrt{3}} = (0, 1.00314, 0.5, -1.49790)$

$\varphi(t) = \alpha_0 + \sqrt{2}\alpha_1 \cos(\pi t) + \sqrt{2}\alpha_2 \cos(2\pi t) + \sqrt{2}\alpha_3 \cos(3\pi t)$

$\varphi(t_k) = x_k \qquad k = 0, 1, 2, 3.$ Demo

Approximating derivatives

Let $x_k = f(t_k)$ and $\varphi(t) = \sum_{\ell=0}^{n-1} \alpha_\ell \cos(\ell \pi t)$

the ~~best~~ approximant of f / interpolant of x.

Then

$$\varphi''(t) = \sum_{\ell=0}^{n-1} -(\ell\pi)^2 \alpha_\ell \cos(\ell \pi t)$$

is an excellent approximation of $\varphi''(t)$.

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y = dct(x)
yp = - π^2 (0,1,...,n-1)^2 .* y
xp = idct(yp)
```

Padding Since $\varphi(t)$ is smooth, we can find more points than n on graph(φ)

Let $\tilde{\alpha} = (\alpha_0, \dots, \alpha_{n-1}, \underbrace{0, 0, \dots, 0}_{m-n})$

$$\boxed{\varphi(t) = \sum_{\ell=0}^{m-1} \tilde{\alpha}_\ell \, \varphi_\ell(t)}$$

But $idct(\tilde{y})$ is contains m points!

Padding: Let data x be given.

$$y = dct(x)$$

$$Y = \sqrt{\frac{m}{n}}(y_0, \dots, y_{n-1}, \underbrace{0, \dots, 0}_{m-n})$$

$$X = idct(Y) \quad \not\equiv \quad T_k = \frac{2k+1}{2m}$$

Demo

Then (T_k, X_k) gives a refinement of $\varphi(t)$

Example Plot 512 points of the interpolant for data $(1, 2, -3, 0)$.

Demo

Discrete sine transform

Let $t_k = \frac{k}{n+1} \qquad k = 1, \dots, n$

and $x_k = f(t_k)$

Define $y = \mathrm{dst}(x) \qquad y_k = \sum_{l=1}^{n} x_l \sin(l\pi t_k)$

$x = \mathrm{idst}(y) \qquad x_k = \frac{2}{n+1} \sum_{l=1}^{n} y_l \sin(l\pi t_k)$

Then $\varphi(t) = \sum_{l=1}^{n} \alpha_l c_l \sin(l\pi t) \qquad \alpha = \frac{\sqrt{2}}{n+1} y$

is the unique sine interpolant / best approximant for (t_k, x_k).

Discrete Fourier Transform (FFT)

Let $\omega_n = e^{-2\pi i/n} = \cos\left(\frac{2\pi}{n}\right) - i\sin\left(\frac{2\pi}{n}\right)$

Given $x = (x_0, \ldots, x_{n-1}) \in \mathbb{C}^n$

$y = \mathrm{fft}(x)$ where $y_k = \sum_{j=0}^{n-1} x_j \omega_n^{kj}$

as with the dct/dst this is a linear transformation.

$x = \mathrm{ifft}(x)$ where $x_k = \frac{1}{n} \sum_{j=0}^{n-1} y_k \omega_n^{-kj}$

Interpolation $t_k = \frac{k}{n}$ $k = 0, \ldots, n-1$

$x = (x_0, \ldots, x_{n-1})$, $y = \mathrm{fft}(x)$

Then $\varphi(t) = \sum_{j=0}^{n-1} \frac{y_j}{n} e^{2\pi i j t}$

is the unique best approx / interpolant

$x_k = \varphi(t_k)$

Complex structure for real data

assume $x \in \mathbb{R}^n$, $y = \text{fft}(x)$ $t_j = \frac{j}{n}$

Then $y_0 \in \mathbb{R}$, $y_k = \overline{y_{n-k}}$ $k = 1, \dots, n-1$

consider

Demo `fft(randn(10,1))` & `fft(randn(9,1))`.

$$\varphi(t) = \sum_{j=0}^{n/2} a_j \cos(2\pi j t) + \sum_{j=1}^{n/2-1} b_j \sin(2\pi j t)$$

$a_0 = \frac{1}{n} y_0$ $a_{n/2} = \frac{1}{n} y_{n/2}$ $j = 1, \dots, \frac{n}{2}-1$

$a_j = \frac{2}{n} \mathrm{Re}\, y_j$ $b_j = -\frac{2}{n} \mathrm{Im}\, y_j$

So the unique interpolant ie

$$x_k = \varphi(t_k) \qquad k = 0, \dots, n-1$$

Differentiation Let n be even

$$\varphi'(t) = \sum -2\pi j\, a_j \sin(2\pi j t) + \sum 2\pi j \cos(2\pi j t)$$

Algorithm

$y = fft(x)$

$yp = d .* y$ where

$d = 2\pi\left(0, i, 2i, \dots, \left(\frac{n}{2}-1\right)i, 0, -\left(\frac{n}{2}-1\right)i, \dots, -2i, -i\right)$

$xp = ifft(yp)$

(t_k, xp_k) approximates $f'(t_k)$ where $f(t_k) = x_k$

Demo

Padding

$y = fft(x)$

$$Y = \frac{m}{n}\Big(\underbrace{y_0, \dots, \frac{y_{n/2}}{2}}_{n/2}, \underbrace{0, \dots, 0}_{m-n-1 \text{ zeros}}, \frac{y_{n/2}}{2}, \underbrace{y_{n/2+1}, \dots, y_{n-1}}_{n/2}\Big)$$

$X = ifft(Y)$ is a refinement of $\varphi(t)$

on points $T_k = \frac{k}{m}$ $k = 0, \dots, m-1$

Demo of periodicpadding.m

Nonlinearities and aliasing

assume that $f(t)$ approximated using $(\alpha_0, \dots, \alpha_{n-1})$

$$\varphi(t) = \sum_{\ell=0}^{n-1} \alpha_\ell \varphi_\ell(t)$$

and we want to find the first n terms of

$$(\varphi(t))^p = \sum_{\ell=0}^{\infty} \gamma_\ell \varphi_\ell(t)$$

Incomplete method

$$
\begin{aligned}
y &= \sqrt{n}\,\alpha \\
x &= \mathrm{idct}(y) \\
xp &= (x_0^p, x_1^p, \dots, x_{n-1}^p) \\
yp &= \mathrm{dct}(xp)
\end{aligned}
$$

Aliasing illustrated by example

Euler $(e^{\pi i x})^p = e^{p\pi i x} = \cos(p\pi x) + i\sin(p\pi x)$

$$= (\cos \pi x + i \sin \pi x)^p$$

Thus we require pn coefficients to represent the exact p^{th} power, even in the first n terms.

NUMERICAL DEMO

Complete method

$$y = \sqrt{n}\,\alpha$$

$$\underline{Y} = \sqrt{\tfrac{m}{n}}\,(y_0, y_1, \dots, y_{n-1}, \overbrace{0 \dots 0}^{(p-1)n}) \quad \text{PAD}$$

$$\underline{X} = \operatorname{idct}(\underline{Y})$$

$$\underline{X}P = (\underline{X}_0^p, \underline{X}_1^p, \dots, \underline{X}_{p-1}^p)$$

$$\underline{Y}P = \operatorname{dct}(\underline{X}P)$$

$$yp = (\underline{Y}P_0, \underline{Y}P_1, \dots, \underline{Y}P_{n-1})$$

$$\beta = yp / \sqrt{n}$$

Then the β coefficients are exact for the first n terms

ie $$\beta_k = \gamma_k \qquad k = 0, \dots, n-1$$

However with more complicated nonlinearities our error estimates are not as straightforward!