Numerical Methods for Computational Science and Engineering

Autumun Semester 2018, Week 5

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Principle Component Analysis (PCA)

Important for:
- dimensionality reduction
- trend analysis
- data classification

Example:

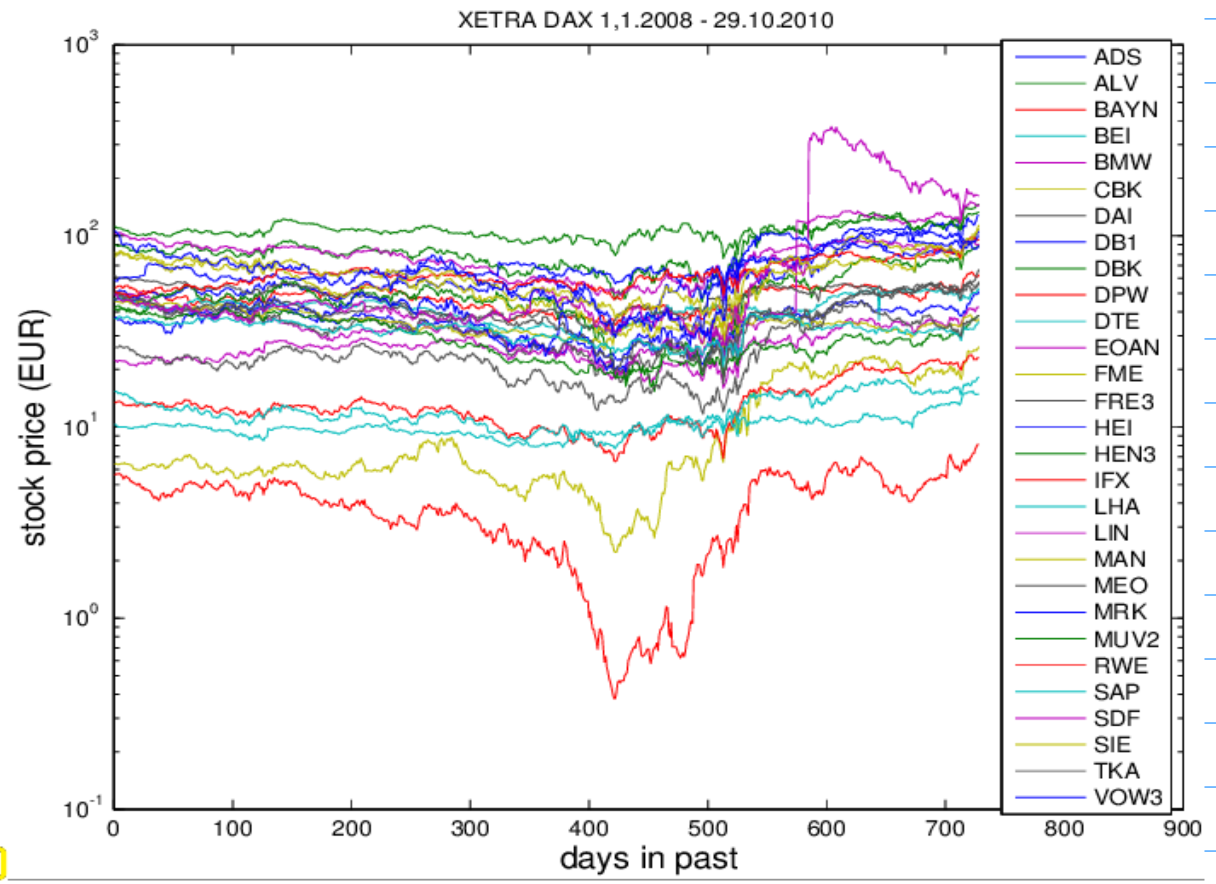


Fig. 106

Is there an underlying trend in the price development?

Each stock price as a vector $a_j \in \mathbb{R}^m$

$j = 1, \dots, n$ (n stocks)

$$A = [a_1 \ a_2 \ \dots \ a_n] \in \mathbb{R}^{m,n}$$

Trend $\hat{=}$ There are a few vectors $\tilde{u}_1, \dots, \tilde{u}_p$, $p \ll n$,
(strict sense)
s.t. $a_j \in \operatorname{span}\{\tilde{u}_1, \dots, \tilde{u}_p\}$
for all $j \in \{1, \dots, n\}$
(and $\tilde{u}_1, \dots, \tilde{u}_p$ orthonormal)

$$\underbrace{\text{This would mean: } \quad \mathcal{R}(A) \subseteq \operatorname{span}\{\tilde{u}_1, \dots, \tilde{u}_p\} \Rightarrow \operatorname{rank}(A) = p}_{\text{unrealistic scenario}}$$

Stock prices for example: small random fluctuations in the stock prices

More realistic scenario instead:

Can we find orthonormal vectors $\tilde{u}_1, \dots, \tilde{u}_p$ s.t.

$\forall j \in \{1, \dots, n\}$: $a_j \in \operatorname{span}\{\tilde{u}_1, \dots, \tilde{u}_p\}$ + "small perturbation"

This means: Stock prices <u>approximately</u> follow a trend

Find an (approximate) trend by exploiting the SVD of A.

$$A = U \Sigma V^T$$

$$\Big[\underset{\substack{\uparrow \\ a_j}}{\ } \ A \ \Big] = \sigma_1 \big[\, u_1 \,\big] \Big[\underset{\substack{\uparrow \\ (v_1)_j}}{\ } v_1^T \Big] + \dots + \sigma_n \big[\, u_n \,\big] \Big[\underset{\substack{\uparrow \\ (v_n)_j}}{\ } v_n^T \Big]$$

Each a_j is a linear combination of $u_1, \dots, u_n$

[Recall: $\{u_1, \dots, u_n\}$ ONB for column space of A]

Vectors v_i carry weights of this linear combination:

$$a_j = (\sigma_1 (v_1)_j)\, u_1 + (\sigma_2 (v_2)_j)\, u_2 + \dots + (\sigma_n (v_n)_j)\, u_n$$

In the unrealistic scenario of rank$(A) = p \ll n$:

last non-zero sing. value

SVD: $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H$ satisfies $\sigma_1 \geq \sigma_2 \geq \dots \sigma_p > \sigma_{p+1} = \dots = \sigma_{\min\{m,n\}} = 0$, orthonormal *trend* vectors $\underbrace{(\mathbf{U})_{:,1}, \dots, (\mathbf{U})_{:,p}}$.

More realistic scenario:

last significant sing. val.

SVD: $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^H$ satisfies $\sigma_1 \geq \sigma_2 \geq \dots \sigma_p \gg \sigma_{p+1} \approx \dots \approx \sigma_{\min\{m,n\}} \approx 0$, orthonormal *trend* vectors $(\mathbf{U})_{:,1}, \dots, (\mathbf{U})_{:,p}$.

pronounced gap

This means: "$\mathcal{R}(A)$ is almost p-dimensional"

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_p u_p v_p^T$$
$$+ \sigma_{p+1} u_{p+1} v_{p+1}^T + \dots + \sigma_n u_n v_n^T$$

comparably small

log scale

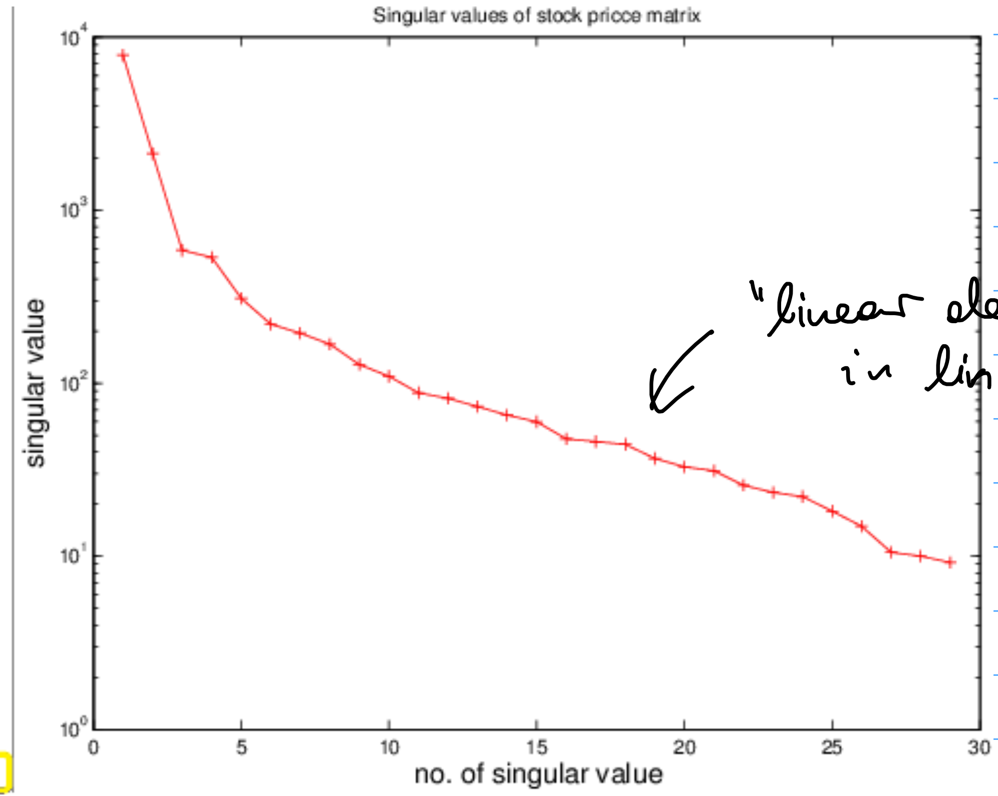


Fig. 121

lin-log plot

"linear decay" in lin-log-scale

$\Downarrow$

exponential decay (in lin-lin-scale)

linear scale

Common criterion:

$$p = \min\left\{ q : \sum_{j=1}^{q} \sigma_j^2 \geq (1-\tau) \sum_{j=1}^{n} \sigma_j^2 \right\} \qquad \tau \ll 1$$

$\rightarrow$ the sum of the first p σ_j^2's is almost as large as the sum over all σ_j^2's.

Example: Classification of measured data

measured data: voltage -vs.- current in diodes

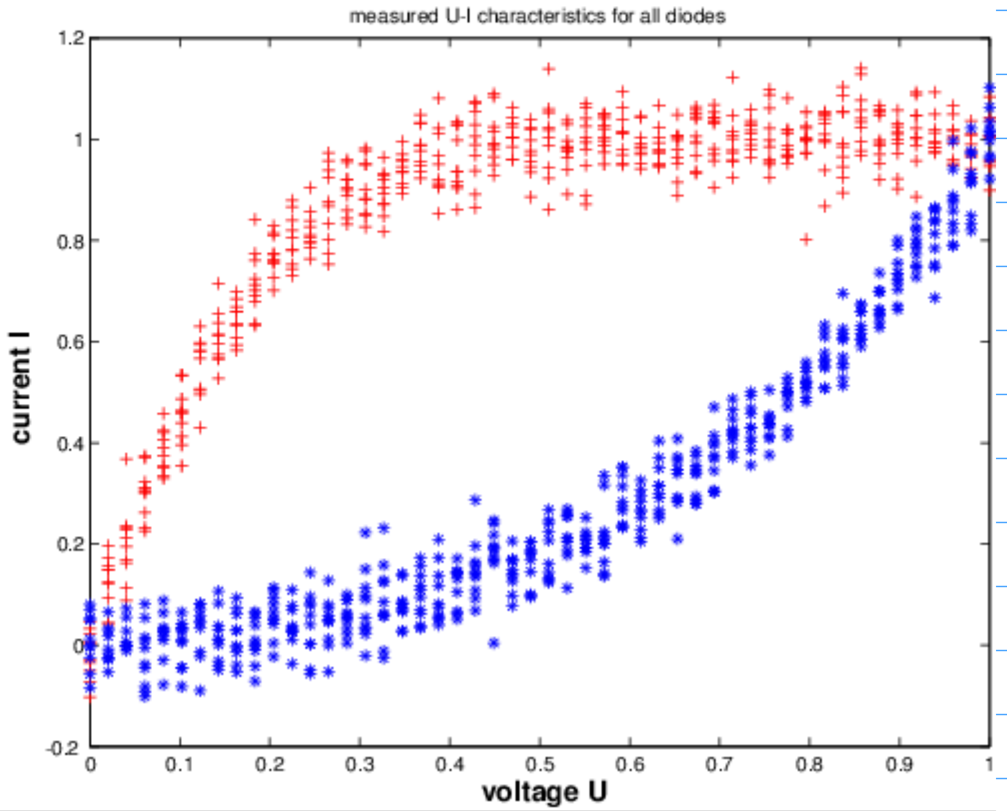


Fig. 109

How many types of diodes $\rightarrow$ consider SVD

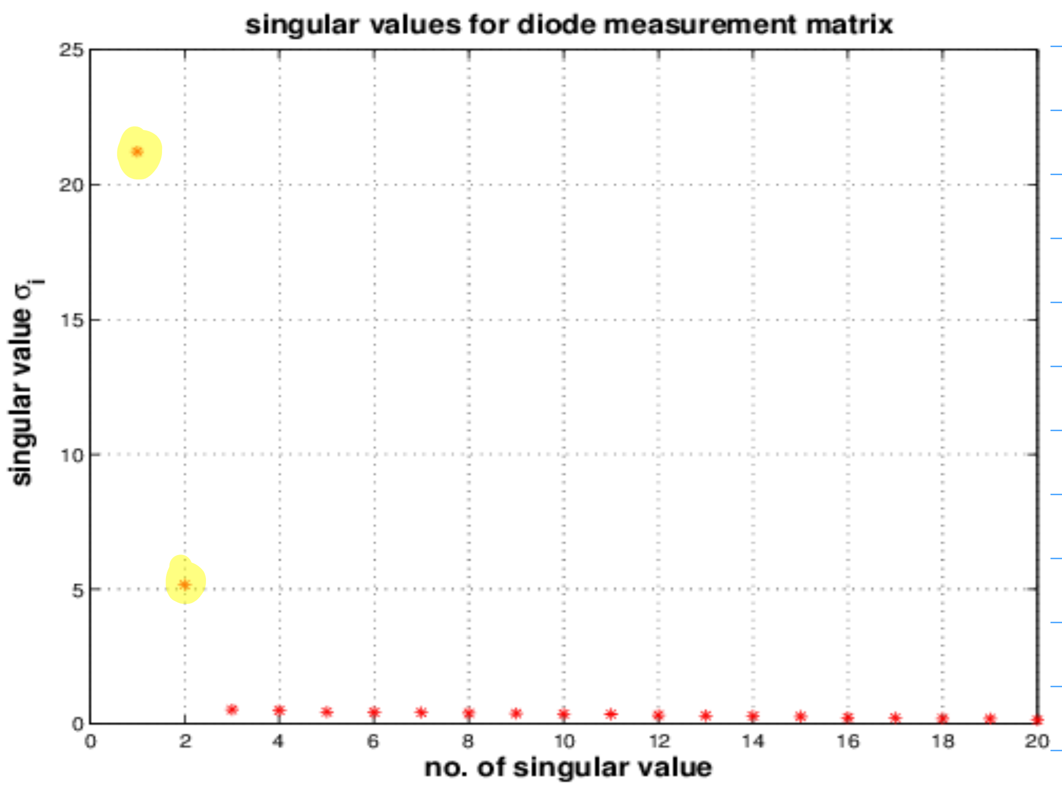


Fig. 113

2 dominant sing values

→ 2 groups in voltage-vs-current behavior

→ this suggest: 2 types of diodes

4. Filtering Algorithms

↓

applying an operation ("filter") to a signal, an image, etc. to analyze / transmit the signal.

signal processing: time-discrete signals as sequences

$$(\ldots, 0, 0, x_0, x_1, x_2, \ldots, x_{n-1}, 0, 0, \ldots)$$

(sampling time-continuous signals)

time-cont. signal: $X(t)$ $\quad t \in [0, T]$

time-discrete signal: $x_j = X(j \cdot \underbrace{\Delta t}_{\text{spacing between 2 samples}})$

$$x = [x_0, x_1, \ldots, x_{n-1}]^T \in \mathbb{R}^n$$

$$n \cdot \Delta t \leq T$$

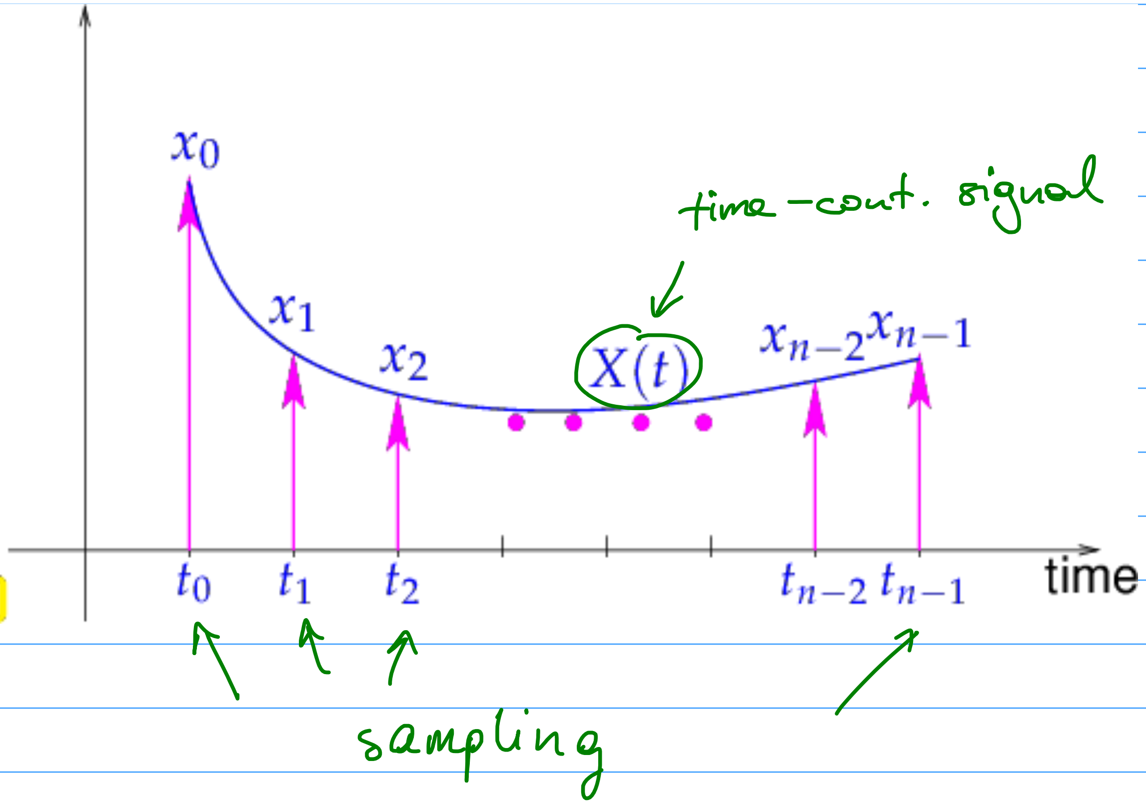


Fig. 127

In general: signal $\hat{=}$ bounded sequence

$$\ell^\infty(\mathbb{Z}) = \Big\{ \underbrace{(x_j)_{j\in\mathbb{Z}}}_{\text{sequence}} : \sup_{j\in\mathbb{Z}} |x_j| < \infty \Big\}$$

4.1 Discrete convolutions (⇝ operating on sequences)

Filters or channels (as in wireless communication)

<u>LT-FIR filters</u>:

Channel/filter: mapping $F: \ell^\infty(\mathbb{Z}) \to \ell^\infty(\mathbb{Z})$

$$F\big((x_j)_{j\in\mathbb{Z}}\big) = (y_j)_{j\in\mathbb{Z}}$$

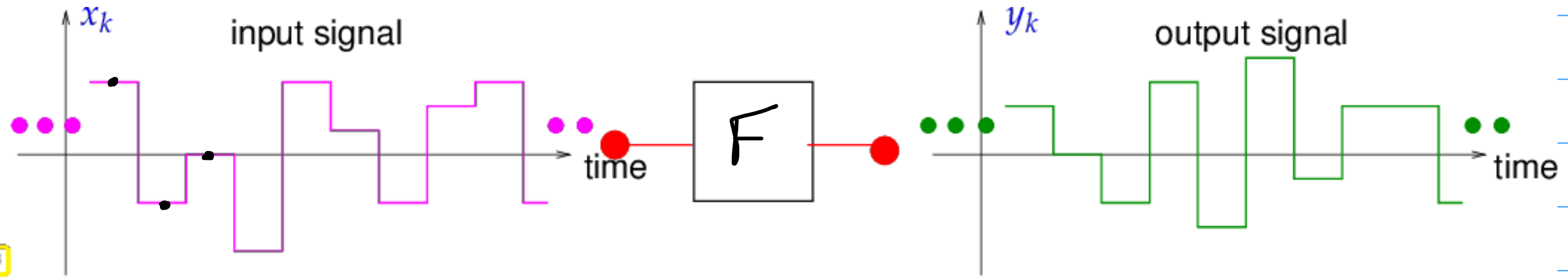


Fig. 128

Properties of F?

- <u>finite</u>: Every finite-length signal $(x_j)_{j\in\mathbb{Z}}$ has a finite-length output $F((x_j)_{j\in\mathbb{Z}})$

- time-invariant:

time-shift of the input & then filter applied

= apply filter & then time-shift output

time-shift operator $S_k : \ell^\infty(\mathbb{Z}) \to \ell^\infty(\mathbb{Z})$

$$S_k\left((x_j)_{j\in\mathbb{Z}}\right) = (x_{j-k})_{j\in\mathbb{Z}}$$

time-invariant:

$$F\left(S_k\left((x_j)_{j\in\mathbb{Z}}\right)\right) = S_k\left(F\left((x_j)_{j\in\mathbb{Z}}\right)\right)$$

- linear:

$$F\Big(\underbrace{\alpha\cdot(x_j)_{j\in\mathbb{Z}} + \beta\cdot(y_j)_{j\in\mathbb{Z}}}_{\text{linear comb. of 2 seq.}}\Big) = \alpha\cdot F\left((x_j)_{j\in\mathbb{Z}}\right) + \beta\cdot F\left((y_j)_{j\in\mathbb{Z}}\right)$$

- causal: output only depends on past & present inputs, not future:

If $x_j = 0 \;\; \forall j \le M \Rightarrow F\left((x_j)_{j\in\mathbb{Z}}\right)_k = 0$
$\forall\, k \le M$

At index k: output only takes into account $x_1, \dots, x_k$

Impulse response:

Analogue: Matrix $\hat{=}$ describing action of a linear map $\mathbb{R}^n \longrightarrow \mathbb{R}^m$ through its action on unit vectors e_j

$$Ae_1 = (A)_{:,1} \qquad Ae_j = (A)_{:,j}$$

Now in the same spirit:

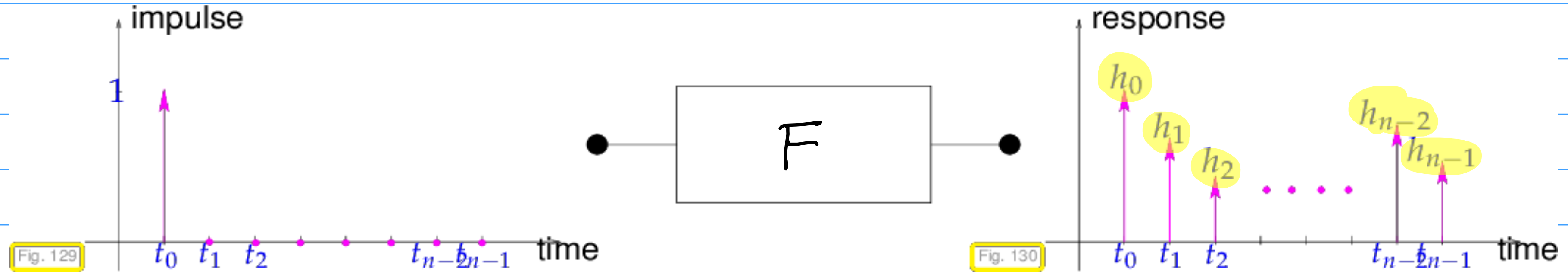
describe filters through their action on "impulses"

$\hat{=}$ "unit sequences"

How does F respond to the input signal

$(\dots, 0, 0, 1, 0, 0, 0, \dots)$ "unit impulse"

$\uparrow$ 0-th entry



We can write $(\dots, 0, 0, 1, 0, 0, 0, \dots)$

$$= (\delta_{j,0})_{j \in \mathbb{Z}}$$

$$\delta_{j,l} = \begin{cases} 1 & j = l \\ 0 & \text{otherwise} \end{cases}$$

$$h_k := F((\delta_{j,0})_{j \in \mathbb{Z}})_k$$

Impulse response $\hat{=}$ "building block"

$\rightarrow$ can build response $F((x_j)_{j \in \mathbb{Z}})$ out of these building blocks

Impulse response $(\dots, 0, 0, h_0, h_1, \dots, h_{m-1}, 0, 0, \dots)$

m: length of the filter

order of the filter

$$F((\delta_{j,0})_{j \in \mathbb{Z}}) = (\dots, 0, 0, \underset{\substack{\uparrow \\ \text{0-th index}}}{h_0}, h_1, \dots, h_{m-1}, 0, 0, \dots)$$

$$F((\underset{\substack{\uparrow \\ \text{shifted unit impulse (shifted by } k)}}{\delta_{j,k}})_{j \in \mathbb{Z}}) = (\dots, 0, 0, \underset{\substack{\uparrow \\ k\text{-th index}}}{h_0}, h_1, \dots, h_{m-1}, 0, 0, \dots)$$

How to use impulse response?

Any finite signal $(x_j)_{j\in\mathbb{Z}} = (\dots, 0, x_0, x_1, \dots, x_{n-1}, 0, \dots)$ is a linear combination of shifted impulses:

$$(x_j)_{j\in\mathbb{Z}} = \sum_{k=0}^{n-1} x_k \cdot \underbrace{(\delta_{j,k})_{j\in\mathbb{Z}}}_{\text{just a basis!}}$$

$$= \sum_{k=0}^{n-1} x_k \cdot \underbrace{S_k}_{\text{time-shift by } k} \left((\delta_{j,0})_{j\in\mathbb{Z}} \right)$$

Response of $(x_j)_{j\in\mathbb{Z}}$?

$$F((x_j)_{j\in\mathbb{Z}}) = F\left(\sum_{k=0}^{n-1} x_k \cdot S_k\left((\delta_{j,0})_{j\in\mathbb{Z}} \right) \right)$$

$$\underset{\text{linearity}}{=} \sum_{k=0}^{n-1} x_k \cdot F\left(S_k\left((\delta_{j,0})_{j\in\mathbb{Z}} \right) \right)$$

$$\underset{\text{time-invariance}}{=} \sum_{k=0}^{n-1} x_k \, S_k \Big(\underbrace{F((\delta_{j,0})_{j\in\mathbb{Z}})}_{\text{impulse response}} \Big)$$

$$(\dots, 0, h_0, \dots, h_{m-1}, 0, \dots)$$

$$(y_j)_{j\in\mathbb{Z}} = F((x_j)_{j\in\mathbb{Z}})$$

$$\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ \\ y_{n+m-2} \end{bmatrix} = x_0 \begin{bmatrix} h_0 \\ h_1 \\ \vdots \\ h_{m-1} \\ 0 \\ \vdots \\ 0 \end{bmatrix} + x_1 \begin{bmatrix} 0 \\ h_0 \\ h_1 \\ \vdots \\ h_{m-1} \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \dots + x_{n-1} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ h_0 \\ \vdots \\ h_{m-1} \end{bmatrix}$$

$$\Rightarrow F((x_j)_{j\in\mathbb{Z}})_k = y_k = \sum_{j=0}^{n-1} x_j h_{k-j}$$

$k = 0, \dots, m+n-2$ $\qquad h_j = 0$ for $j<0$, $j \geq m$

Output is a linear combination of shifted impulse responses

Maximal duration of output:

$$\underbrace{n}_{\text{length of signal}} + \underbrace{m}_{\text{length of filter}} - 1$$

Example:

signal: $(x_j)_{j\in\mathbb{Z}} = (\ldots, 0, 0, 3, 1, 2, 4, 0, 0, \ldots)$ $\quad n = 4$

filter (impulse response): $(\ldots, 0, 0, 1, 1, 2, 3, 1, 0, 0, \ldots)$ $\quad m = 5$

Output $F((x_j)_{j\in\mathbb{Z}})$?

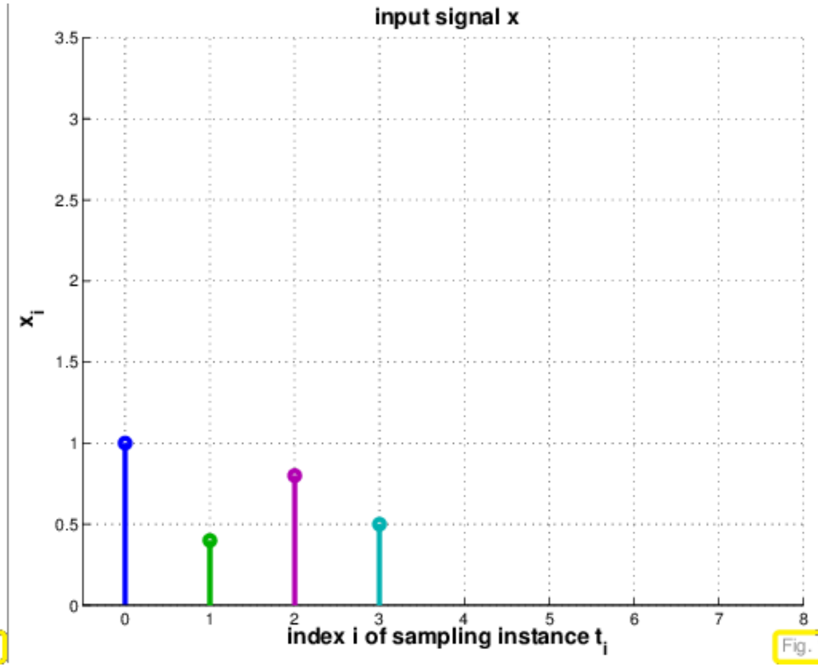


Fig. 131

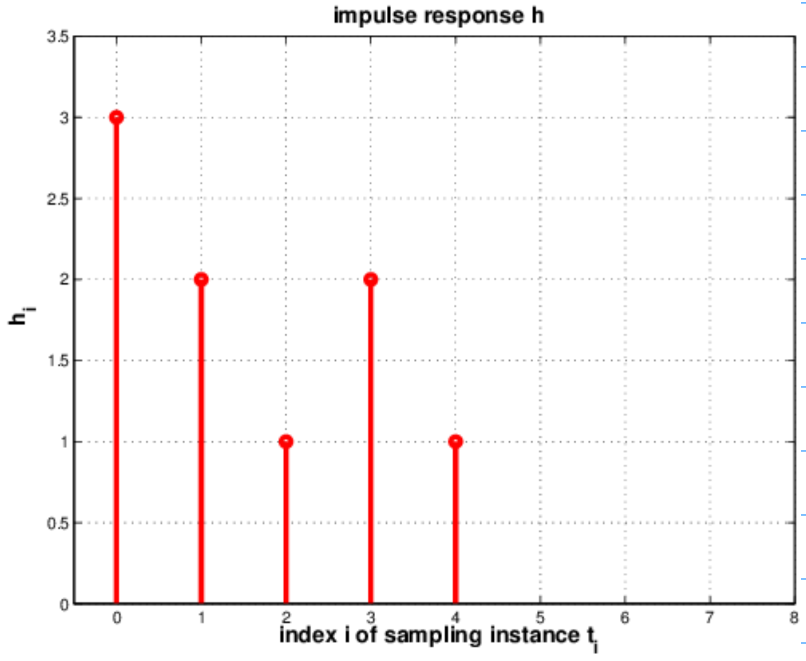


Fig. 132

$x = (\ldots, 0, x_0, \ldots, x_3, 0, \ldots)$ $\quad n = 4$

$h = (\ldots, 0, h_0, \ldots, h_4, 0, \ldots)$ $\quad m = 5$

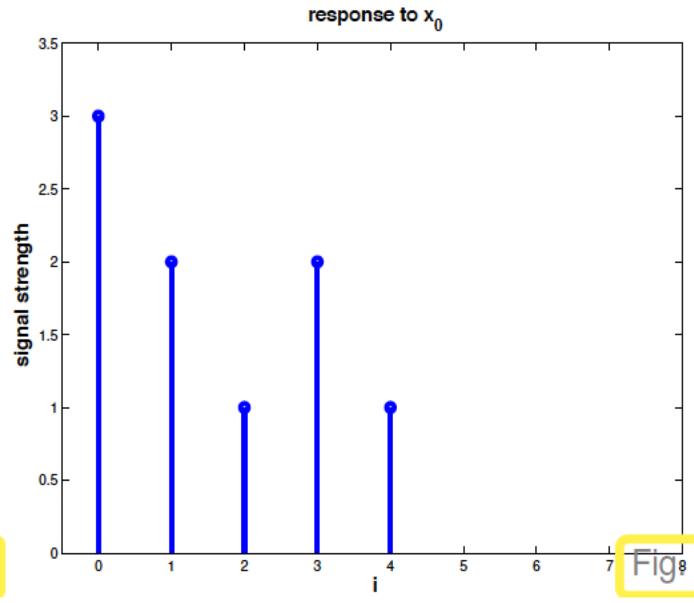


Fig 134

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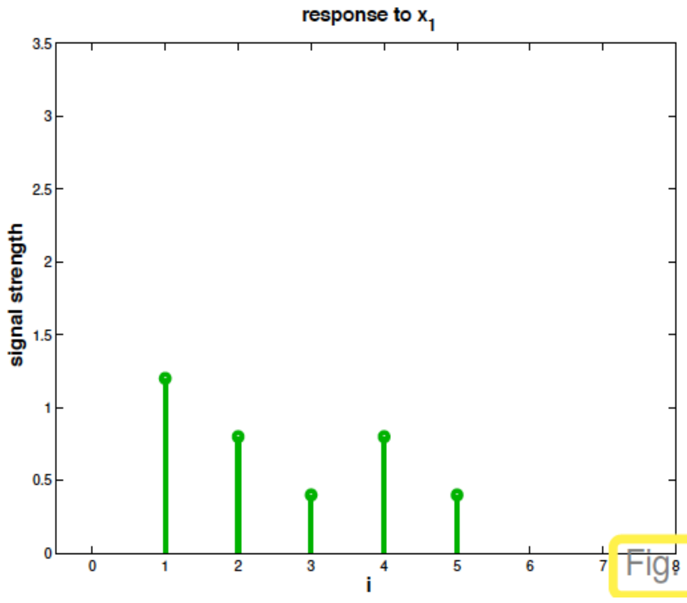

Fig 135

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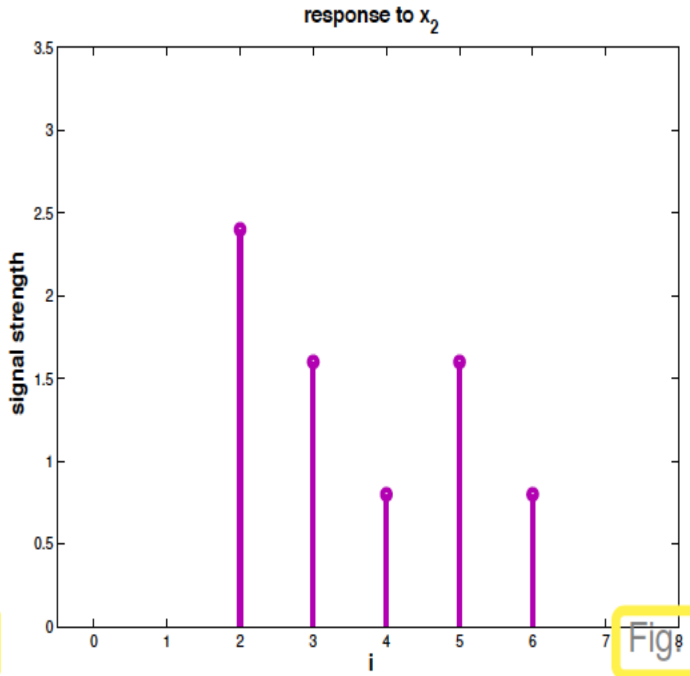

Fig 136

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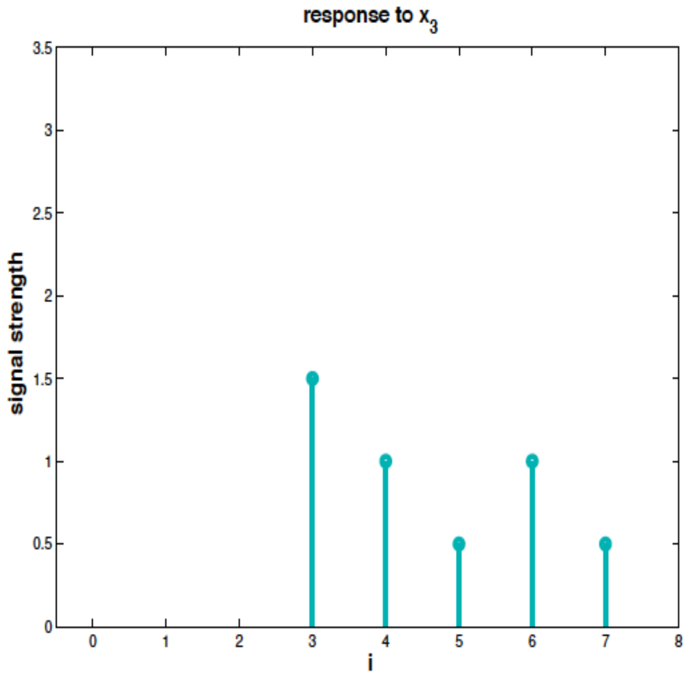


Add up all the responses:

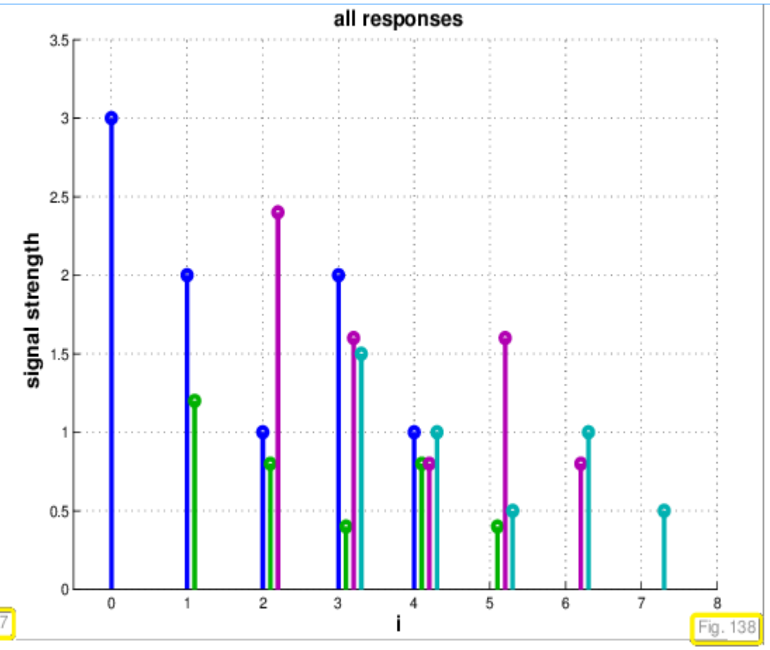


Fig. 137

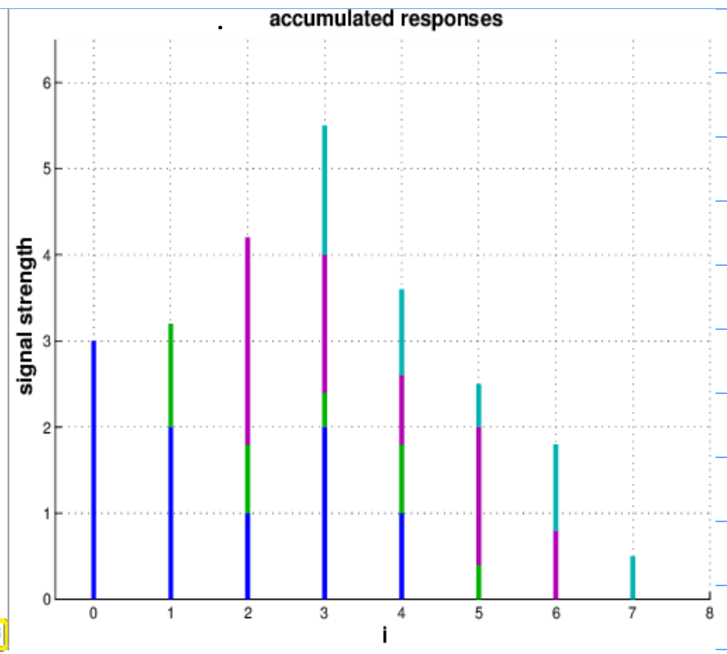


Fig. 138

For finite length signals:

- Represent $x = (\dots, 0, x_0, \dots, x_{n-1}, 0, \dots)$ by a vector $\underline{x} = [x_0, \dots, x_{n-1}]^T \in \mathbb{R}^n$

- Represent filter as a linear mapping $F: \mathbb{R}^n \to \mathbb{R}^{m+n-1}$

Here: filter of length m

$$\begin{bmatrix} y_0 \\ \vdots \\ \vdots \\ \\ y_{m+n-2} \end{bmatrix} = \begin{bmatrix} h_0 & 0 & \cdots & \cdots & 0 \\ h_1 & h_0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ h_{m-1} & & & \ddots & h_0 \\ 0 & \ddots & & & h_1 \\ \vdots & \ddots & \ddots & & \vdots \\ 0 & & \ddots & \ddots & \\ 0 & \cdots & \cdots & 0 & h_{m-1} \end{bmatrix} \begin{bmatrix} x_0 \\ \vdots \\ \vdots \\ \vdots \\ x_{n-1} \end{bmatrix}$$

$\Rightarrow$ Representation of an LT-FIR filter as a matrix.

Can we exploit the special matrix structure?

Recall: $F((x_j)_{j\in\mathbb{Z}})_k = \sum_{j\in\mathbb{Z}} x_j h_{k-j}$

This operation is called (linear) discrete convolution

of $x = (\ldots, 0, x_0, \ldots, x_{n-1}, 0, \ldots)$

with $h = (\ldots, 0, h_0, \ldots, h_{m-1}, 0, \ldots)$

Definition (discrete convolution):

For 2 finite sequences $f, g \in \ell^\infty(\mathbb{Z})$ their discrete convolution

$$u := f * g \quad (= g * f) \in \ell^\infty(\mathbb{Z})$$

is defined by

$$u_k := \sum_{j\in\mathbb{Z}} f_j g_{k-j} = \sum_{j\in\mathbb{Z}} f_{k-j} g_j$$

Filtering: output $y = x * h$ finite & in $\ell^\infty(\mathbb{Z})$

In the same way:

discrete convolution for vectors:

$$\underline{y} := \underline{x} * \underline{h} \qquad y_k = \sum_{j=0}^{n-1} x_j h_{k-j}$$

$\uparrow$
$\in \mathbb{R}^{m+n-1}$

where $h_j = 0$ for $j \notin \{0, \dots, m-1\}$

(convention)

y_k is the inner product of x and time-shifted (by k) and reversed h.

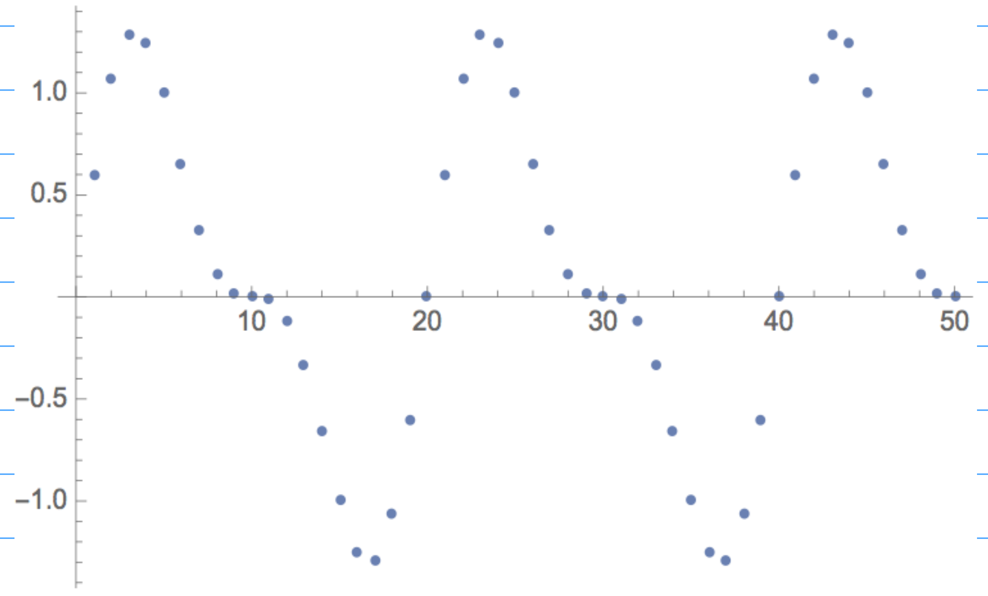
Circular / periodic convolution:

Goal: It turns out that periodic convolution is "easier" ($\rightsquigarrow$ convolution theorem)

So ultimately: describe linear convolution from before as periodic convolution

Filtering of periodic signal

$$x_j = x_{j+n} \qquad \forall j \in \mathbb{Z} \quad \text{(period of length } n\text{)}$$



$$y_k = \sum_{j\in\mathbb{Z}} x_j h_{k-j}$$

$$= \sum_{j\in\mathbb{Z}} x_{k-j} h_j \qquad \text{(then: } y \text{ is also } n\text{-periodic)}$$

$$= \sum_{j=0}^{n-1} \underbrace{\left(\sum_{\ell\in\mathbb{Z}} h_{j+\ell n}\right)}_{\text{periodic summation}} x_{k-j}$$

$$p_j^{n} := \sum_{\ell\in\mathbb{Z}} h_{j+\ell n}$$

where $h = (\ldots, 0, h_0, \ldots, h_{m-1}, 0, \ldots)$

Note:

$$p_{j+n} = \sum_{\ell\in\mathbb{Z}} h_{j+n+\ell n} = \sum_{\ell\in\mathbb{Z}} h_{j+\ell n} = p_j$$

$$\sum_{\ell\in\mathbb{Z}} h_{j+(\ell+1)n}$$

More generally: $p_{j+kn} = p_j \quad \forall\, k\in\mathbb{Z}$

$\Rightarrow$ $p^{(n)}$ is n-periodic as well

$$y_k = \sum_{j=0}^{n-1} p_j x_{k-j} = \sum_{j=0}^{n-1} p_{k-j} x_j \qquad k\in\mathbb{Z}$$

Definition 4.1.7 (Discrete periodic convolution)**.** The *discrete periodic convolution* of two n-periodic sequences $(p_k)_{k\in\mathbb{Z}}$, $(x_k)_{k\in\mathbb{Z}}$ yields the n-periodic sequence:

$$(y_k) := (p_k) *_n (x_k) \quad , \quad y_k := \sum_{j=0}^{n-1} p_{k-j} x_j = \sum_{j=0}^{n-1} x_{k-j} p_j \,, \quad k\in\mathbb{Z}\,.$$

$$y_0 = p_0 x_0 + p_{-1} x_1 + \ldots + p_{-(n-1)} x_{n-1}$$

$$= p_0 x_0 + p_{n-1} x_1 + \ldots + p_1 x_{n-1}$$

$$y_1 = p_1 x_0 + p_0 x_1 + \ldots + p_{-(n-2)} x_{n-1}$$

$$= p_1 x_0 + p_0 x_1 + \ldots + p_2 x_{n-1}$$

$$
\begin{bmatrix} y_0 \\ \vdots \\ \\ \\ \vdots \\ y_{n-1} \end{bmatrix}
=
\underbrace{\begin{bmatrix}
p_0 & p_{n-1} & p_{n-2} & \cdots & & \cdots & p_1 \\
p_1 & p_0 & p_{n-1} & & & & \vdots \\
p_2 & p_1 & p_0 & \ddots & & & \\
\vdots & & \ddots & \ddots & \ddots & & \\
& & & \ddots & \ddots & \ddots & \\
\vdots & & & & \ddots & \ddots & p_{n-1} \\
p_{n-1} & p_{n-2} & & & & p_1 & p_0
\end{bmatrix}}_{=:\mathbf{P}}
\begin{bmatrix} x_0 \\ \vdots \\ \\ \\ \vdots \\ x_{n-1} \end{bmatrix}.
$$

very special structure

Circulant matrix

Definition 4.1.8 (Circulant matrix). A matrix $\mathbf{C} = [c_{ij}]_{i,j=0}^{n-1} \in \mathbb{K}^{n,n}$ is *circulant* if an only if there exists an n-periodic sequence $(p_k)_{k\in\mathbb{Z}}$ such that:

$$c_{ij} = p_{j-i}\,, 0 \le i,j \le n-1$$

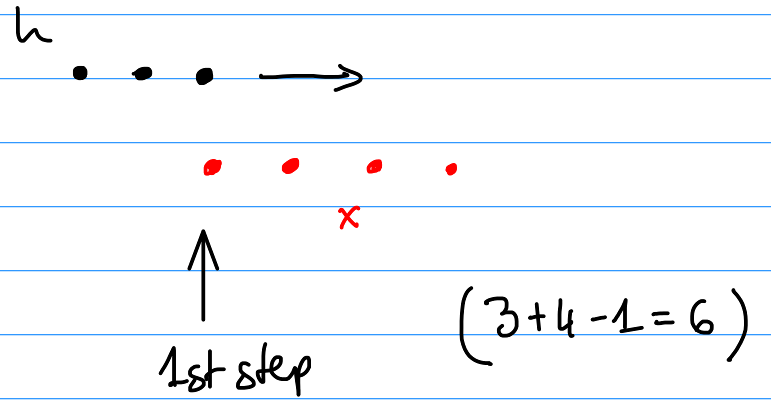
Circulant matrix: Diagonal & all subdiagonals are constant

↳ determined by $\mathbf{p} = [p_0, \cdots, p_{n-1}]^T$

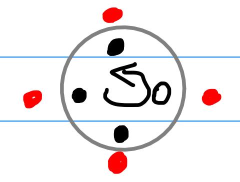
Later: We will exploit the nice property of circulant matrices (i.e. their relation to the Fourier matrix)

But first: Can we interpret linear convolution as $\underbrace{\text{periodic convolution}}_{\text{multiplication by a circulant matrix}}$

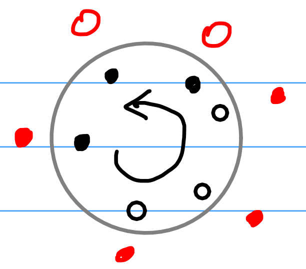
Linear convolution



Periodic convolution (length 4)



this is not equivalent!



period length 6

this is the periodic convolution equivalent to the linear conv.

$\Rightarrow$ Discrete linear convolution of

$$\underline{x} = [x_0, \dots, x_{n-1}]^T \quad \text{and}$$

$$\underline{h} = [h_0, \dots, h_{m-1}]^T$$

$$y_k = (\underline{x} * \underline{h})_k = \sum_{j=0}^{n-1} x_j h_{k-j} \qquad k = 0, \dots, m+n-2$$

y has length $m+n-1$

↳ to "fit" this in a periodic setting requires period of length $L := m+n-1$

zero-pad $\underline{x}$ to length L

$$\underline{x}^L = [x_0, \dots, x_{n-1}, 0, \dots, 0]^T \in \mathbb{R}^L$$

x^L periodic extension of $\underline{x}^L$

↓

sequence

$$h = (\dots, 0, h_0, \dots, h_{m-1}, 0, \dots) \quad \text{s.t.}$$

$$\hookrightarrow \quad p_j = \sum_{l \in \mathbb{Z}} h_{j+lL} = h_{j+kL} \quad \leftarrow \in \{0, \dots, m-1\}$$

↑ L is large enough

$$\underline{h}^L = [h_0, \dots, h_{m-1}, 0, \dots, 0]^T$$

p is periodic extension of $\underline{h}_L$

$$\boxed{y^L = x^L *_L p}$$

k-th entry of y^L = k-th entry of y

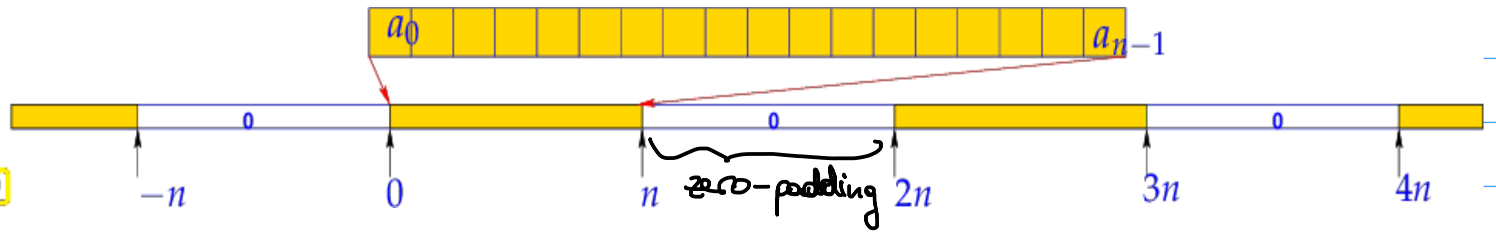


Fig. 139

a is a signal of length n
zero-padded to length $2n$
and then periodized

$$\begin{bmatrix} y_0 \\ \vdots \\ \vdots \\ y_{L-1} \end{bmatrix} = \begin{bmatrix} p_0 & p_{L-1} & \cdots & p_1 \\ p_1 & p_0 & & \vdots \\ \vdots & p_1 & & \vdots \\ \vdots & \vdots & & \vdots \\ p_{L-1} & p_{L-2} & & p_0 \end{bmatrix} \begin{bmatrix} x_0 \\ \vdots \\ x_{n-1} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$L = m + n - 1$$

length of h (m) ; length of x (n)

In terms of h:

$$\begin{bmatrix} y_0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ y_{L-1} \end{bmatrix} = \underbrace{\begin{bmatrix} h_0 & 0 & \cdots & h_{m-1} & h_{m-2} & \cdots & h_1 \\ h_1 & h_0 & & 0 & h_{m-1} & & \vdots \\ \vdots & h_1 & & \vdots & 0 & & \vdots \\ \vdots & \vdots & & 0 & \vdots & & h_{m-1} \\ h_{m-1} & \vdots & & h_0 & 0 & & 0 \\ 0 & h_{m-1} & & \vdots & h_0 & & \vdots \\ \vdots & 0 & & \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots & \vdots & & 0 \\ 0 & 0 & & h_{m-2} & h_{m-3} & \cdots & h_0 \end{bmatrix}}_{\in \mathbb{R}^{L,L}} \begin{bmatrix} x_0 \\ \vdots \\ \vdots \\ x_{n-1} \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix}$$

circulant matrix

Example:

Signal: $\underline{x} = [2, 1, 3, 2]^T$

Filter: $\underline{h} = [1, 1, 2]^T$

1. 4-periodic convolution?
2. 6-periodic convolution?

1. $y^4 = x^4 *_4 p^4$

$$x^4 = (\dots, 2, 1, 3, 2, 2, 1, 3, 2, 2, 1, 3, 2, \dots)$$

$$p^4 = (\dots, 1, 1, 2, 0, 1, 1, 2, 0, 1, 1, 2, 0, \dots)$$

Exercise: Compute y^4

2. 6-periodic convolution

$y^6 = x^6 *_6 p^6$

$$x^6 = (\dots, 2, 1, 3, 2, 0, 0, 2, 1, 3, 2, 0, 0, 2, \dots)$$

$$p^6 = (\dots, 1, 1, 2, 0, 0, 0, 1, 1, 2, 0, 0, 0, 1, \dots)$$

Exercise: Compute y^6

Consider the case in which the period is shorter than the length of h:

$\underline{x} = [2, 1]^T$ $\quad x = (\ldots, 2, 1, 2, 1, 2, 1, \ldots)$

$\underline{h} = [1, 1, 2]^T$

$y^2 = x^2 *_2 p^2$

$p = (\ldots, \underset{h_0 + h_2}{3}, \underset{h_1}{1}, 3, 1, 3, 1, \ldots)$