ENGG5781 Matrix Analysis and Computations
Lecture 2: Linear Representations and Least Squares

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Lecture 2: Least Representations and Least Squares

- Part I: linear representations
  - time-series modeling, Vandemonde matrix
  - basis representation
  - discrete-time linear time-invariant systems, Toeplitz matrix, circulant matrix
  - OFDM, localization
- Part II: least squares (LS)
  - projection theorem, orthogonal projection, pseudo-inverse
  - LS by optimization
- Part III: extensions
  - matrix factorization, PCA, matrix completion
  - gradient descent, online algorithms

Main Result

- **Problem:** given $\mathbf{y} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times n}$, solve

$$\min_{\mathbf{x} \in \mathbb{R}^n} \ \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 \qquad \text{(LS)}$$

  - find an $\mathbf{x}$ whose residual $\mathbf{r} = \mathbf{y} - \mathbf{A}\mathbf{x}$ is the smallest in the Euclidean sense

- **Solution:** suppose that $\mathbf{A}$ has full column rank. The solution to (LS) is unique and is given by

$$\mathbf{x}_{\text{LS}} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$$

  - if $\mathbf{A}$ is semi-orthogonal, the solution is simplified to $\mathbf{x}_{\text{LS}} = \mathbf{A}^T\mathbf{y}$
  - unless specified, in this lecture we will assume $\mathbf{A}$ to have full column rank without further mentioning

Part I: Linear Representations

Linear Representation

There are numerous applications in which we deal with a representation

$$\mathbf{y} = \mathbf{A}\mathbf{x},$$

or

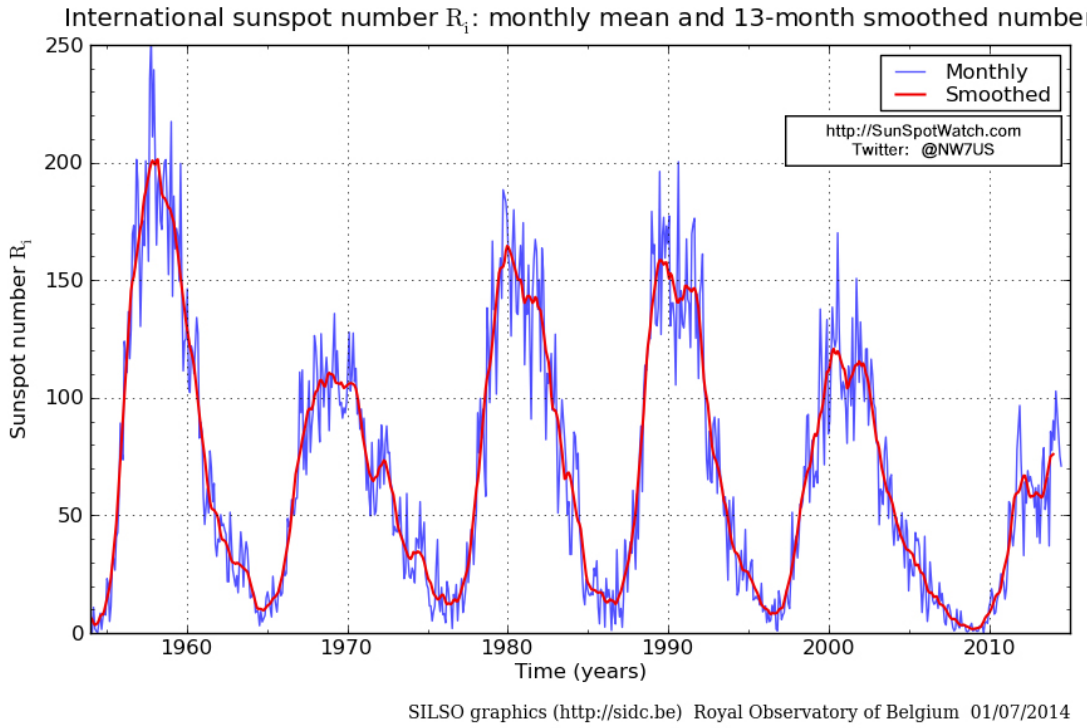
$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{v},$$

where $\mathbf{y}$ is given; $\mathbf{A}$ is given or stipulated; $\mathbf{x}$ is to be determined; $\mathbf{v}$ is noise or error.

Time Series

- let y_t, $t = 0, 1, \ldots$, be a real-valued time series.

- examples: speech signal, music, stock market index, real-time seismic waveforms, air quality index (AQI), sunspot counts, ...



Sunspot time series. Source: http://sunspotwatch.com

Time Series

- one can analyze a time series using model-free techniques such as Fourier transform
  - by model-free, we mean that we make little assumptions on the time series
- we can also apply a model
- model-based approaches exploit problem natures and can work very well—assuming that you choose a right model for your data

Harmonic Model for Time Series

- Harmonic model:

$$y_t = \sum_{i=1}^{k} A_i r_i^t \cos(2\pi f_i t + \phi_i) + v_t, \quad t = 0, 1, \ldots$$

  for some positive integer k and for some $A_i > 0$, $r_i > 0$, $f_i \in \left[-\frac{1}{2}, \frac{1}{2}\right)$, $\phi_i \in [0, 2\pi)$, $i = 1, \ldots, k$; v_t is noise or modeling error.

  - (A_i, r_i, f_i, ϕ_i)'s are model parameters and unknown
  - k is called the model order; also unknown but we can plug a guess number

- we can use the *Hilbert transform*[1] to convert y_t to a complex time series

$$\tilde{y}_t = \sum_{i=1}^{k} A_i r_i^t e^{\boldsymbol{\jmath} 2\pi f_i t + \phi_i} + \tilde{v}_t = \sum_{i=1}^{k} \alpha_i z_i^t + \tilde{v}_t,$$

  where $\alpha_i = A_i e^{\boldsymbol{\jmath}\phi_i}$, $z_i = r_i e^{\boldsymbol{\jmath} 2\pi f_i}$.

[1] call `hilbert` on MATLAB

Harmonic Model for Time Series

- suppose z_i's are known, and the observation time window is T. Then,

$$\underbrace{\begin{bmatrix} \tilde{y}_0 \\ \tilde{y}_1 \\ \tilde{y}_2 \\ \vdots \\ \tilde{y}_{T-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_k \\ z_1^2 & z_2^2 & \cdots & z_k^2 \\ \vdots & & & \vdots \\ z_1^{T-1} & z_2^{T-1} & \cdots & z_k^{T-1} \end{bmatrix}}_{=\mathbf{A}} \underbrace{\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_k \end{bmatrix}}_{=\mathbf{x}} + \underbrace{\begin{bmatrix} \tilde{v}_0 \\ \tilde{v}_1 \\ \tilde{v}_2 \\ \vdots \\ \tilde{v}_{T-1} \end{bmatrix}}_{=\mathbf{v}}$$

  - we can estimate the amplitude-phase coefficients α_i's from $\{\tilde{y}_t\}$ via LS, given information of the frequencies f_i's and the damping coefficients r_i's

Vandemonde Matrix

A matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ is said to be Vandemonde if it takes the form

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_n \\ z_1^2 & z_2^2 & \cdots & z_n^2 \\ \vdots & & & \vdots \\ z_1^{m-1} & z_2^{m-1} & \cdots & z_n^{m-1} \end{bmatrix},$$

where $z_i \in \mathbb{C}$, $i = 1, \ldots, n$, are called the roots of the Vandemonde matrix.

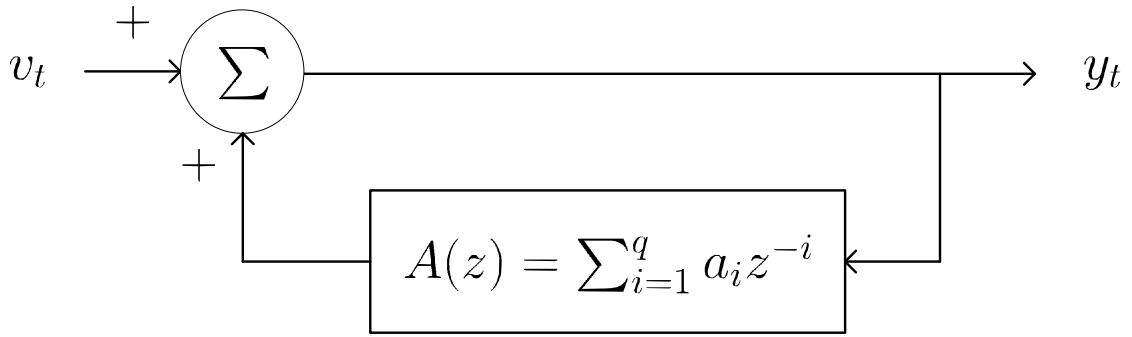
- Fact: a Vandemonde $\mathbf{A}$ has full rank if its roots are distinct; i.e., $z_i \neq z_j$ for all i, j with $i \neq j$
  - Vandemonde matrices possess a stronger linear independence property: if we pick *any* k columns of $\mathbf{A}$, with $k \leq n$, they are always linearly independent.

Autoregessive Model for Time Series

- Autoregressive (AR) model:

$$y_t = a_1 y_{t-1} + a_2 y_{t-2} + \ldots + a_q y_{t-q} + v_t, \quad t = 0, 1, \ldots$$

for some coefficient $\mathbf{a} \in \mathbb{R}^q$ and for some positive integer (or model order) q.



  - model y_t as being related to its past values in a linear manner
  - also called the all-pole model in signals and systems

Autoregessive Model for Time Series

- Prediction: suppose $\mathbf{a}$ is known and we have the time series up to time $t-1$.
  - we may predict the present from the past via

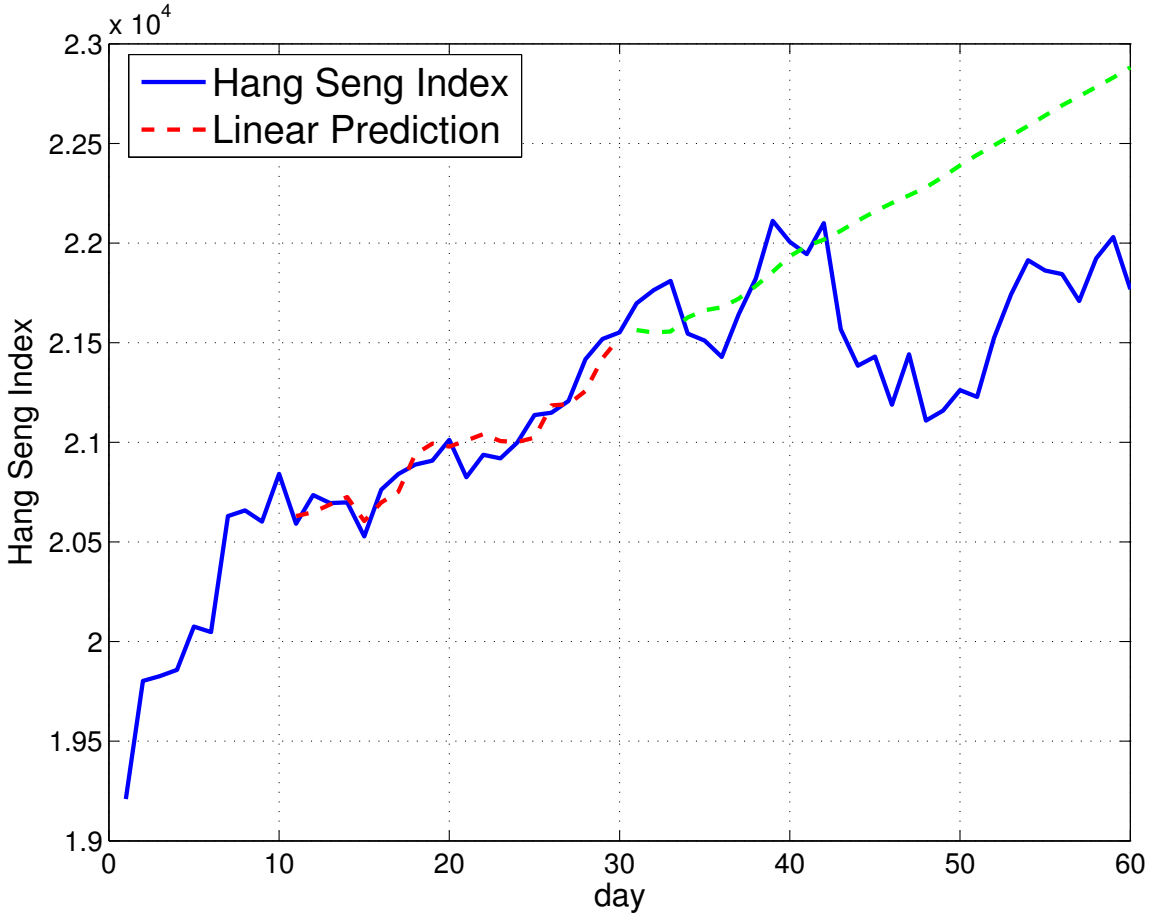
$$\hat{y}_t = a_1 y_{t-1} + a_2 y_{t-2} + \ldots + a_q y_{t-q}$$

  - we may also try to predict the future by recursively running

$$\hat{y}_{t+d} = a_1 \hat{y}_{t+d-1} + a_2 \hat{y}_{t+d-2} + \ldots + a_q \hat{y}_{t+d-q}, \quad d = 1, 2, \ldots$$

  where we denote $\hat{y}_{t-i} = y_{t-i}$ for $i = 1, \ldots, q$.

Toy Demo.: Predicting Hang Seng Index



blue: Hang Seng Index during a certain time period.

red: training phase; $\hat{y}_t = \sum_{i=1}^{q} a_i y_{t-i}$; $\mathbf{a}$ is obtained by LS; $q = 10$.

green: prediction phase; $\hat{y}_{t+d} = \sum_{i=1}^{q} a_i \hat{y}_{t+d-i}$.

Autoregessive Model for Time Series

- let $T+1$ be the observation time window. We have

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_q \\ \vdots \\ \vdots \\ y_T \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} y_0 & & & \\ y_1 & y_0 & & \\ \vdots & & \ddots & \\ y_{q-1} & \cdots & y_1 & y_0 \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ y_{T-q+1} & \cdots & \cdots & y_{T-1} \end{bmatrix}}_{=\mathbf{A}} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_q \end{bmatrix}}_{=\mathbf{x}} + \underbrace{\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_q \\ \vdots \\ \vdots \\ v_T \end{bmatrix}}_{=\mathbf{v}}$$

  - we can estimate the AR coefficients a_i's from $\{y_t\}_{t=0}^{T}$ via LS

Moving Average Model for Time Series

- Moving Average (MA) model:

$$y_t = b_1 v_t + b_2 v_{t-1} + \ldots + b_p v_{t-p+1}, \quad t = 0, 1, \ldots$$

  for some coefficient $\mathbf{b} \in \mathbb{R}^p$; p is the model order; v_t is unknown but assumed to be "white."

- not as simple as the AR case; *roughly* speaking we can do this trick:

$$Y(z) = B(z)V(z) \Longrightarrow \underbrace{\frac{1}{B(z)}}_{=A(z)} Y(z) = V(z) \Longrightarrow$$

  convert back in time as AR with many a_i's

  here $X(z)$ denotes the z-transform of x_t.

- one can also do ARMA

- further reading: **[Stoica-Moses'97]**

Polynomial Model for Time Series

- Polynomial model:

$$y_t = a_0 + a_1 t + a_2 t^2 + \ldots + a_p t^p + v_t, \quad t = 0, 1, \ldots,$$

  where $\mathbf{a} \in \mathbb{R}^{p+1}$.

  – $p = 1$: a line, $p = 2$: quadratic, ...

- Interpolation: use $a_0 + a_1 t + a_2 t^2 + \ldots + a_p t^p$ to predict y_t for *any* $t \in \mathbb{R}$

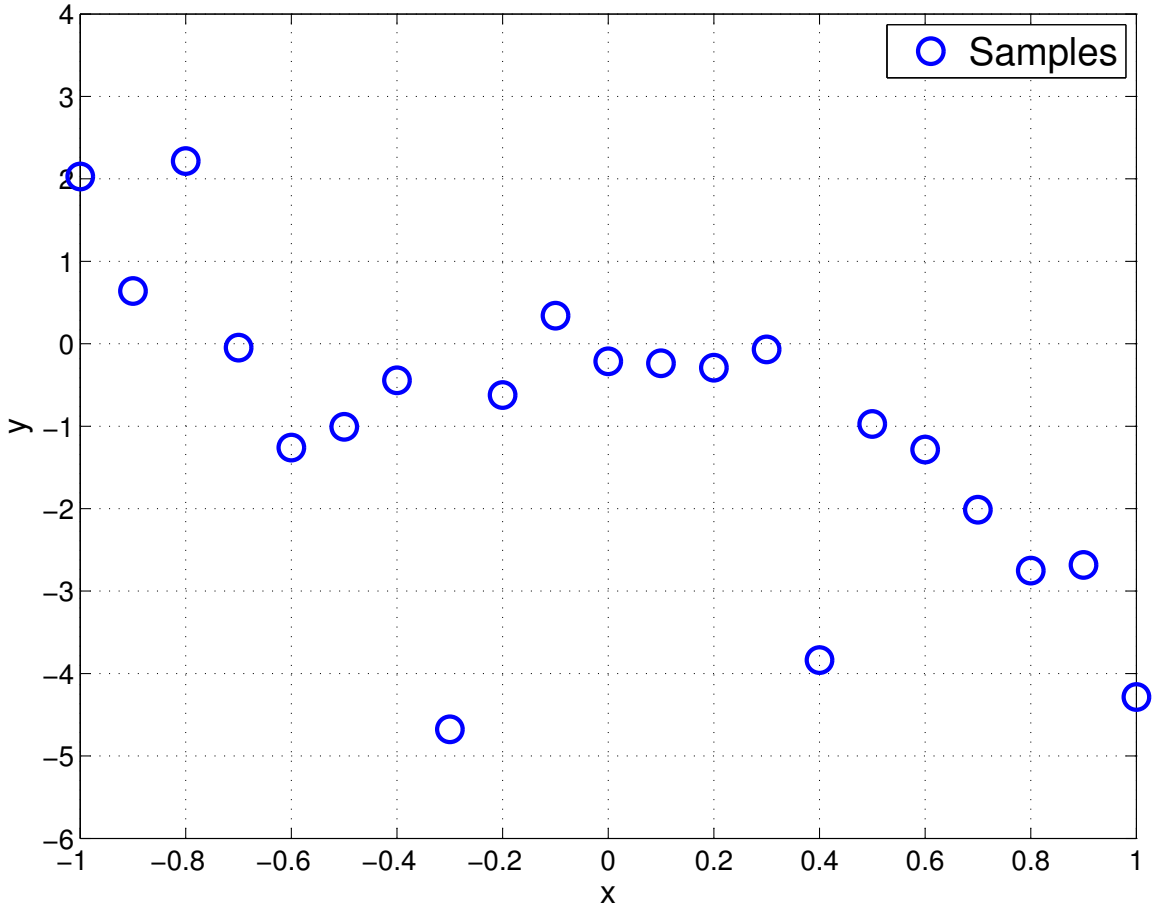
- we have

$$\underbrace{\begin{bmatrix} y_0 \\ \vdots \\ y_t \\ \vdots \\ y_{T-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} 1 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ 1 & t & \cdots & t^p \\ \vdots & & & \vdots \\ 1 & T-1 & \cdots & (T-1)^p \end{bmatrix}}_{=\mathbf{A}} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_p \end{bmatrix}}_{=\mathbf{x}} + \underbrace{\begin{bmatrix} v_0 \\ \vdots \\ v_t \\ \vdots \\ v_{T-1} \end{bmatrix}}_{=\mathbf{v}}$$

  – $\mathbf{A}^T$ is Vandemonde with distinct roots; thus $\mathbf{A}$ has full rank

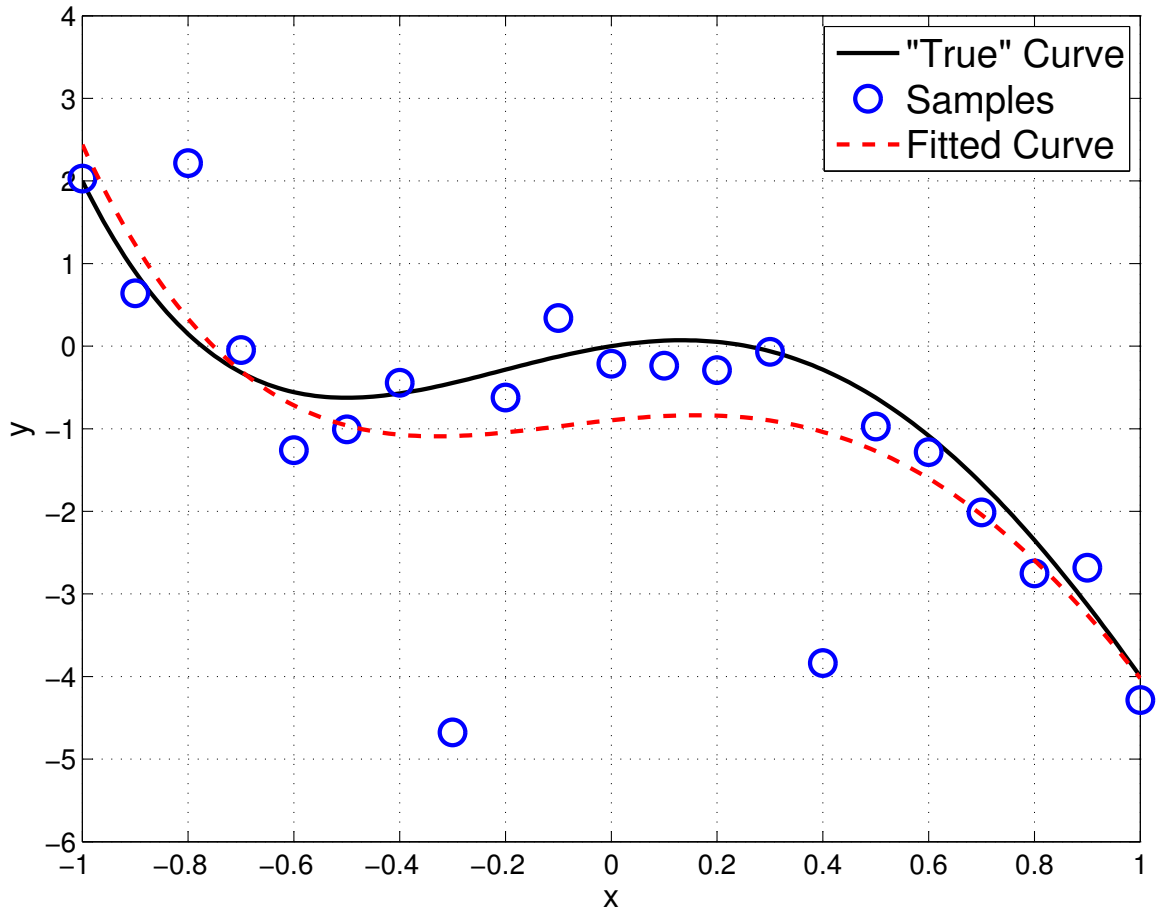
Curve Fitting

Aim: given a set of input-output data pairs $(x_i, y_i) \in \mathbb{R} \times \mathbb{R}$, $i = 1, \ldots, m$, find a function $f(x)$ that fits the data well



Curve Fitting

Like time series, we can apply a polynomial model $f(x) = \sum_{i=0}^{p} a_i x^i$ and use LS



"True" curve: the true $f(x)$; $p = 5$. Fitted curve: estimated $f(x)$; $\mathbf{a}$ obtained by LS; $p = 5$.

Basis Representation

- Aim: represent a given vector $\mathbf{y}$ using a basis $\{\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n\} \subseteq \mathbb{R}^n$:

$$\mathbf{y} = \sum_{i=1}^{n} x_i \boldsymbol{\phi}_i = \boldsymbol{\Phi}\mathbf{x},$$

  where $\mathbf{x}$ is the coefficient

  – we will call $\boldsymbol{\Phi} \in \mathbb{R}^{n \times n}$ a basis matrix or a dictionary

- in particular, we wish $\mathbf{x}$ would be sparse, or approximately sparse in the sense of that $\|\mathbf{x}\|_2^2$ is dominated by a few x_i's

- having a sparse $\mathbf{x}$ is good as it enables compact representation and compression

- $\boldsymbol{\Phi}$ is specifically designed; many designs lead to orthogonal $\boldsymbol{\Phi}$

Basis Representation

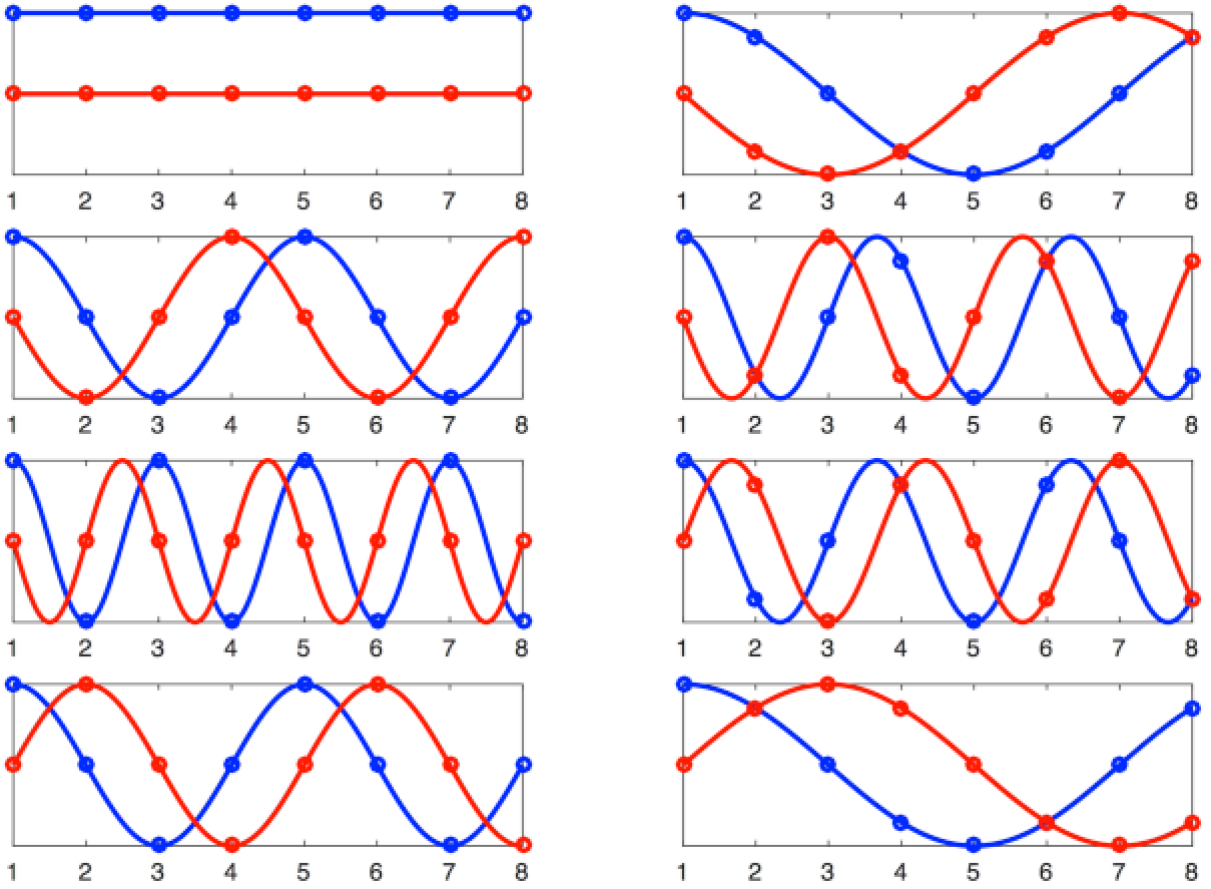
- example: orthonormal Fourier basis

$$\boldsymbol{\phi}_i = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 \\ e^{\boldsymbol{\jmath} 2\pi(i-1)/n} \\ \vdots \\ e^{\boldsymbol{\jmath} 2\pi(n-1)(i-1)/n} \end{bmatrix}, \quad i = 1, \ldots, n.$$

  - $\boldsymbol{\Phi}^H$ is a discrete Fourier transform (DFT) matrix; it can be verified that if we let $\boldsymbol{\Psi} = \boldsymbol{\Phi}^H$ then $\boldsymbol{\psi}_i = \frac{1}{\sqrt{n}}[\ 1\ e^{-\boldsymbol{\jmath} 2\pi(i-1)/n}\ \ldots\ e^{-\boldsymbol{\jmath} 2\pi(n-1)(i-1)/n}\ ]^T$
  - $\boldsymbol{\Phi}$ is an inverse DFT (IDFT) matrix
  - we don't store $\boldsymbol{\Phi}$ physically; we use fast Fourier transform (FFT) and inverse FFT (IFFT) to implement $\mathbf{x} = \boldsymbol{\Phi}^H \mathbf{y}$ and $\mathbf{y} = \boldsymbol{\Phi}\mathbf{x}$, resp.
  - FFT or IFFT complexity: $\mathcal{O}(n \log(n))$

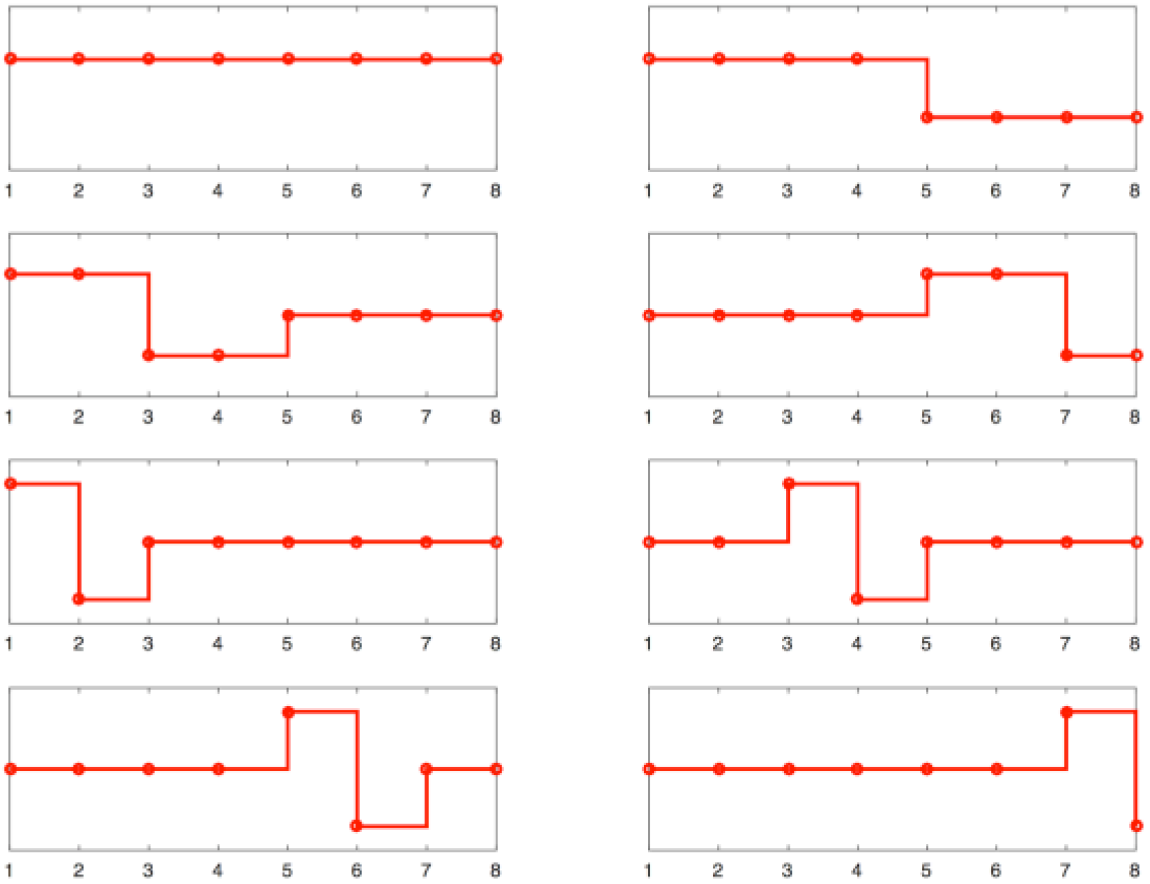
- other basis examples: discrete cosine transform (DCT), Haar, wavelets, ...

Basis Example: DFT Basis



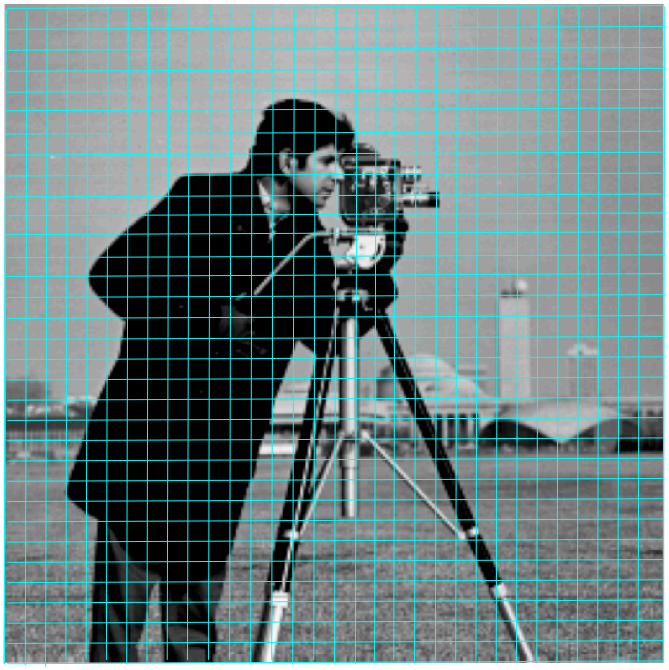
$n = 8$; circles: values of the basis elements; lines: interpolated values for better visualization; blue: real part of the basis elements; red: imaginary part of the basis elements.

Basis Example: Haar Wavelet



$n = 8$; circles: values of the basis elements; lines: interpolated values for better visualization.

Basis Representation Example for Images



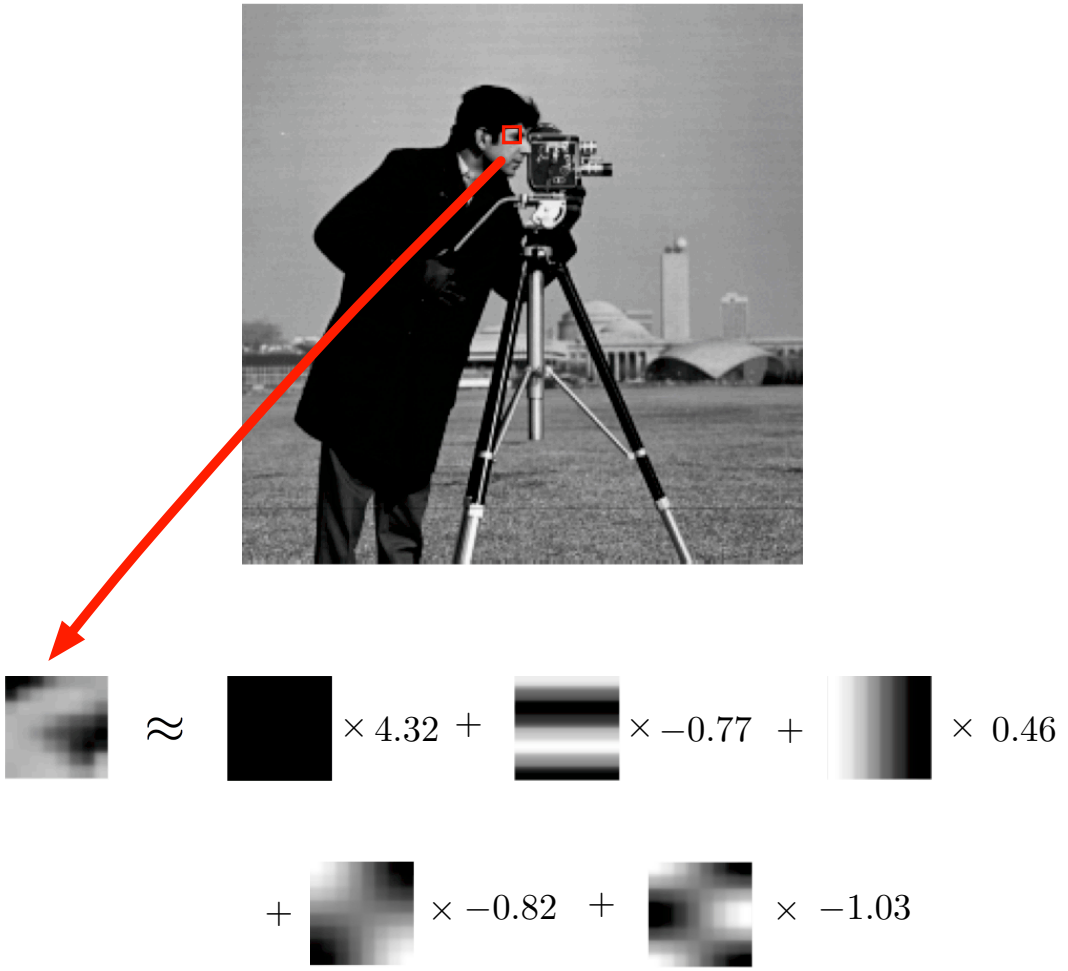
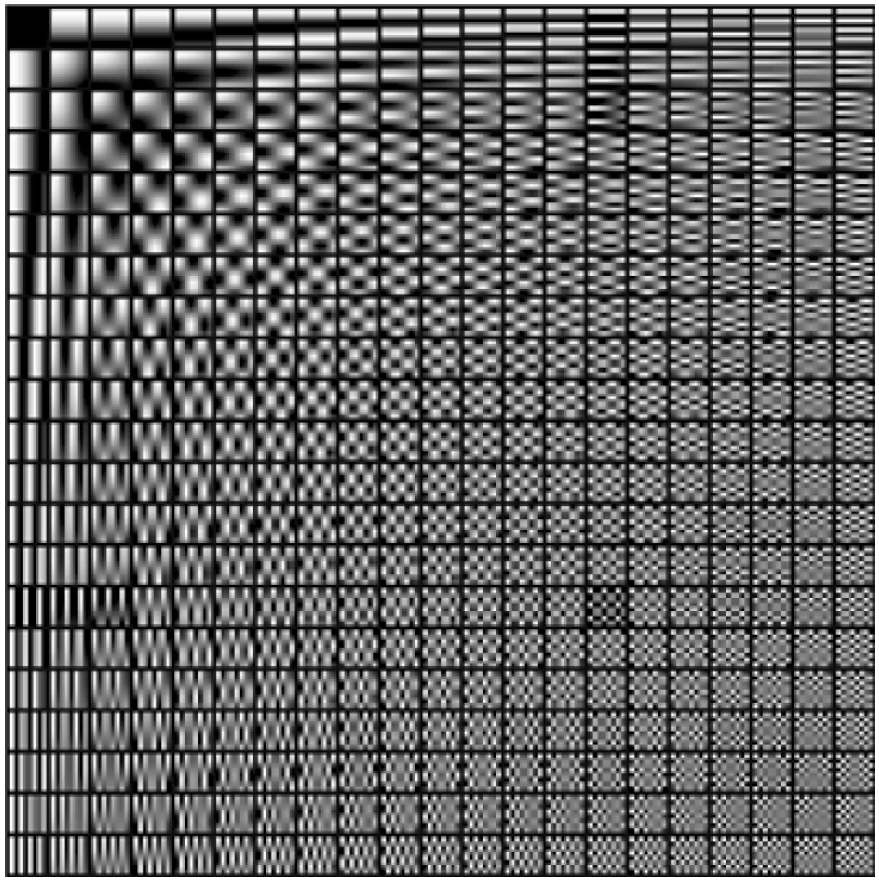
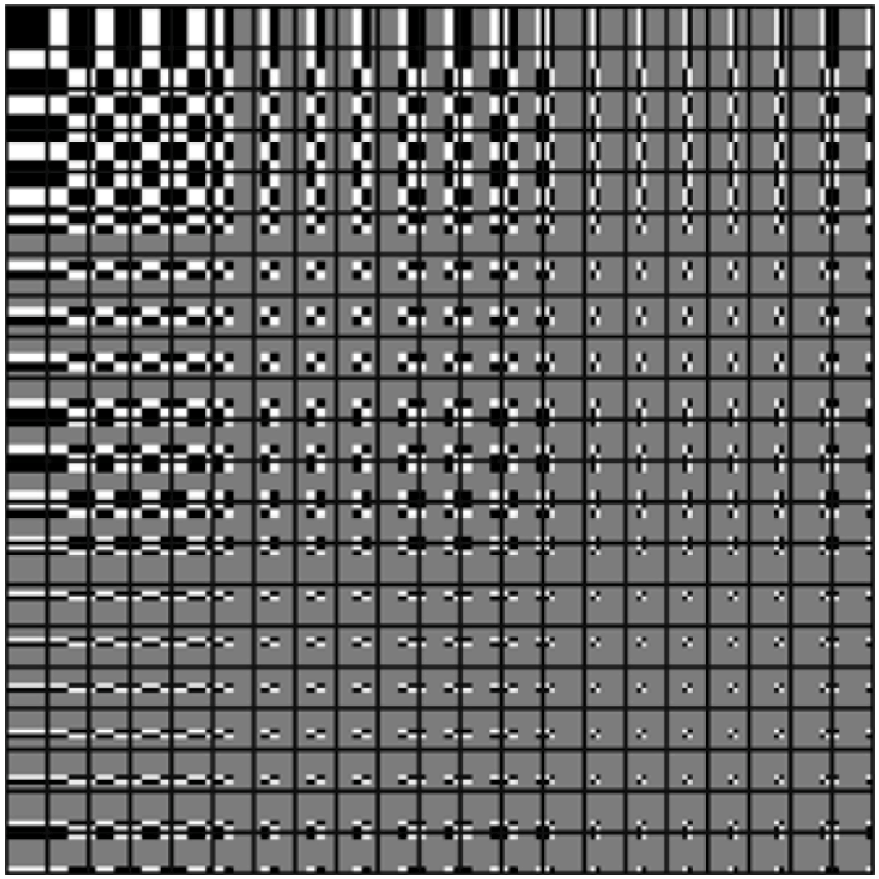


Image representation using a 2D-DCT basis. Left: an image is first cropped into patches, each with a size of 8×8. Right: each patch is represented by a linear combination of basis elements.

Basis Representation Example for Images



(a) 2D DCT dictionary.



(b) 2D Haar wavelet dictionary.

Illustration of the 2D DCT and Haar wavelet dictionaries. Source: **[Aharon-Elad-Bruckstein'06]**. Note that the dictionaries shown are overcomplete.

Discrete-Time Linear Time-Invariant Systems

- consider linear time-invariant system models in discrete-time signal processing:

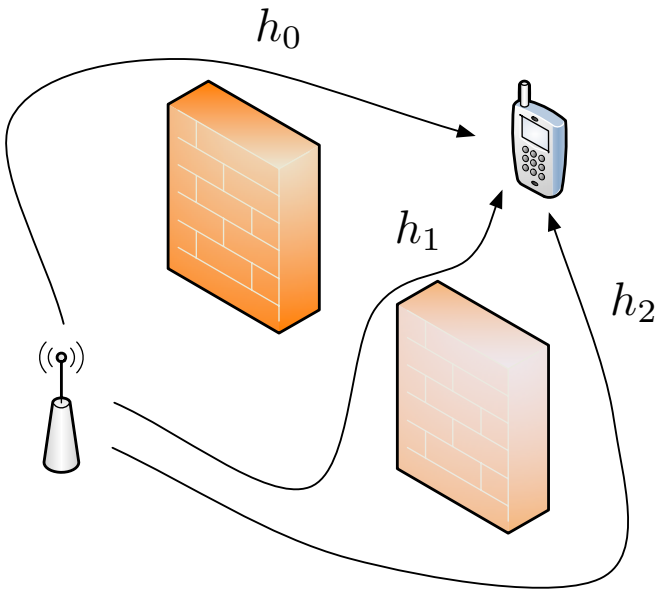
$$y_t = \sum_{i=0}^{p} h_i x_{t-i} + v_t, \quad t = 0, 1, \ldots$$

  where x_t is the input signal; y_t is the output signal; v_t is noise; $\{h_t\}$ is the system impulse response.

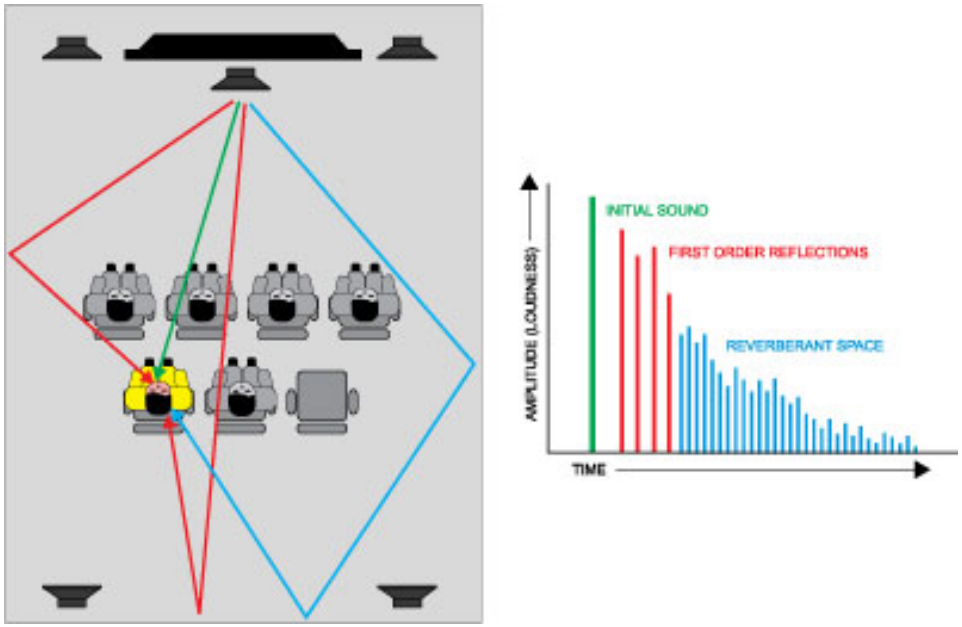
  – some mild assumptions: $\{h_t\}$ is finite in length; $x_t = 0$ for $t = -1, -2, \ldots$

- applications: communications, acoustics, image processing...

Discrete-Time Linear Time-Invariant Systems



(a) multipath propagation in wireless communications.



(b) room acoustics. Picture source: http://acousticsolutions.gr

Discrete-Time Linear Time-Invariant Systems

- System identification: given an input signal block $\{x_t\}_{t=0}^{T-1}$ and an output signal block $\{y_t\}_{t=0}^{T-1}$, find the system impulse response $\{h_t\}_{t=0}^{p}$.
  - applications: channel estimation in communications, identification of acoustic impulse responses,...

- we have

$$\underbrace{\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_p \\ \vdots \\ \vdots \\ y_{T-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} x_0 & & & \\ x_1 & x_0 & & \\ \vdots & & \ddots & \\ x_p & \dots & x_1 & x_0 \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ x_{T-1} & \dots & x_{T-p} & x_{T-1-p} \end{bmatrix}}_{=\mathbf{A}} \underbrace{\begin{bmatrix} h_0 \\ h_1 \\ \vdots \\ h_p \end{bmatrix}}_{=\mathbf{x}} + \underbrace{\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_p \\ \vdots \\ \vdots \\ v_{T-1} \end{bmatrix}}_{=\mathbf{v}}$$

Discrete-Time Linear Time-Invariant Systems

- Deconvolution: given an output signal block $\{y_t\}_{t=0}^{T-1}$ and the system impulse response $\{h_t\}_{t=0}^{p}$, estimate the input signal block $\{x_t\}_{t=0}^{T-1}$
  - applications: equalization in communications, de-reverberation in room acoustics, image deblurring,...

- we have

$$\underbrace{\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_p \\ \vdots \\ \vdots \\ y_{T-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} h_0 & & & & & & \\ h_1 & h_0 & & & & & \\ \vdots & & \ddots & & & & \\ h_p & \dots & h_1 & h_0 & & & \\ & \ddots & & & \ddots & & \\ & & \ddots & & & \ddots & \\ & & & h_p & \dots & h_1 & h_0 \end{bmatrix}}_{=\mathbf{A}\in\mathbb{R}^{T\times T}} \underbrace{\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_p \\ \vdots \\ \vdots \\ x_{T-1} \end{bmatrix}}_{=\mathbf{x}} + \underbrace{\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_p \\ \vdots \\ \vdots \\ v_{T-1} \end{bmatrix}}_{=\mathbf{v}}$$

  - $\mathbf{A}$ is band diagonal and Toeplitz

Toeplitz Matrix

A matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is said to be Toeplitz if it takes the form

$$\mathbf{A} = \begin{bmatrix} h_0 & h_{-1} & \cdots & \cdots & h_{-n+1} \\ h_1 & h_0 & h_{-1} & & \vdots \\ \vdots & h_1 & h_0 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & h_{-1} \\ h_{n-1} & \cdots & \cdots & h_1 & h_0 \end{bmatrix},$$

or $a_{ij} = h_{i-j}$ for all i, j.

- for a general $\mathbf{A} \in \mathbb{R}^{n \times n}$, solving $\mathbf{A}\mathbf{x} = \mathbf{y}$ requires $\mathcal{O}(n^3)$
- for a Teoplitz $\mathbf{A}$, $\mathbf{A}\mathbf{x} = \mathbf{y}$ may be solved in $\mathcal{O}(n^2)$
  - done by exploiting structures; see **[Golub-Van Loan'12]** for details

Circulant Matrix

A matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is said to be circulant if it takes the form

$$\mathbf{A} = \begin{bmatrix} h_0 & h_{n-1} & \dots & \dots & h_1 \\ h_1 & h_0 & h_{n-1} & \dots & h_2 \\ h_2 & h_1 & h_0 & \dots & h_3 \\ \vdots & & & & \vdots \\ \vdots & & & & \vdots \\ h_{n-1} & \dots & \dots & h_1 & h_0 \end{bmatrix}.$$

- for a circulant $\mathbf{A}$, $\mathbf{A}\mathbf{x} = \mathbf{y}$ may be solved in $\mathcal{O}(n \log(n))$

Circulant Matrix

- let $\{\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n\}$ be the DFT basis, and observe that

$$\mathbf{A}\boldsymbol{\phi}_i = \frac{1}{\sqrt{n}} \begin{bmatrix} h_0 & h_{n-1} & \cdots & \cdots & h_1 \\ h_1 & h_0 & h_{n-1} & \cdots & h_2 \\ h_2 & h_1 & h_0 & \cdots & h_3 \\ \vdots & & & & \vdots \\ \vdots & & & & \vdots \\ h_{n-1} & \cdots & \cdots & h_1 & h_0 \end{bmatrix} \begin{bmatrix} 1 \\ e^{\boldsymbol{j}2\pi(i-1)/n} \\ e^{\boldsymbol{j}4\pi(i-1)/n} \\ \vdots \\ \vdots \\ e^{\boldsymbol{j}2\pi(n-1)(i-1)/n} \end{bmatrix}$$

$$= \frac{1}{\sqrt{n}} \underbrace{\sum_{k=0}^{n-1} h_k e^{-\boldsymbol{j}2\pi k(i-1)/n}}_{=d_i} \begin{bmatrix} 1 \\ e^{\boldsymbol{j}2\pi(i-1)/n} \\ e^{\boldsymbol{j}4\pi(i-1)/n} \\ \vdots \\ \vdots \\ e^{\boldsymbol{j}2\pi(n-1)(i-1)/n} \end{bmatrix} = d_i \boldsymbol{\phi}_i.$$

  - note $e^{\boldsymbol{j}2\pi k(i-1)/n} = e^{-\boldsymbol{j}2\pi(n-k)(i-1)/n}$ for any $k \in \{0, 1, \ldots, n-1\}$

Circulant Matrix

- let $\mathbf{D} = \mathrm{Diag}(d_1, \ldots, d_n)$. We have

$$\begin{aligned} \mathbf{A}\boldsymbol{\phi}_i = d_i\boldsymbol{\phi}_i,\ i = 1, \ldots, n \quad &\Longleftrightarrow \quad \mathbf{A}[\ \boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n\ ] = [\ \boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n\ ]\mathbf{D} \\ &\Longleftrightarrow \quad \mathbf{A}\boldsymbol{\Phi} = \boldsymbol{\Phi}\mathbf{D} \\ &\Longleftrightarrow \quad \mathbf{A} = \boldsymbol{\Phi}\mathbf{D}\boldsymbol{\Phi}^H \end{aligned}$$

- Fact (as a summary): a circulant matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ can be decomposed as

$$\mathbf{A} = \boldsymbol{\Phi}\mathbf{D}\boldsymbol{\Phi}^H,$$

where $\boldsymbol{\Phi}$ is the IDFT matrix; $\mathbf{D} = \mathrm{Diag}(d_1, \ldots, d_n)$; $d_i = \sum_{k=0}^{n-1} h_k e^{-\boldsymbol{\jmath} 2\pi k(i-1)/n}$.

  - as will be studied, the above decomposition is an eigendecomposition

Circulant Matrix

- Question: how does a circulant $\mathbf{A}$ help us solve $\mathbf{y} = \mathbf{A}\mathbf{x}$?
  - suppose $d_i \neq 0$ for all i
  - we have $\mathbf{A}^{-1} = \mathbf{\Phi}\mathbf{D}^{-1}\mathbf{\Phi}^H$ and

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{y} = \underbrace{\mathbf{\Phi}\underbrace{(\mathbf{D}^{-1}\overbrace{(\mathbf{\Phi}^H\mathbf{y})}^{\text{FFT}})}_{n \text{ multiplies}}}_{\text{IFFT}}$$

  - complexity: one FFT + n multiplies + one IFFT = $\mathcal{O}(n\log(n))$
    - the above complexity assumes that $d_1, \ldots, d_n$ have been pre-computed; computing $d_1, \ldots, d_n$ requires FFT and the complexity is $\mathcal{O}(n\log(n))$

Circulant Approximation of Linear Time-Invariant Systems

- back to deconvolution, we may approximate the system matrix as being circulant

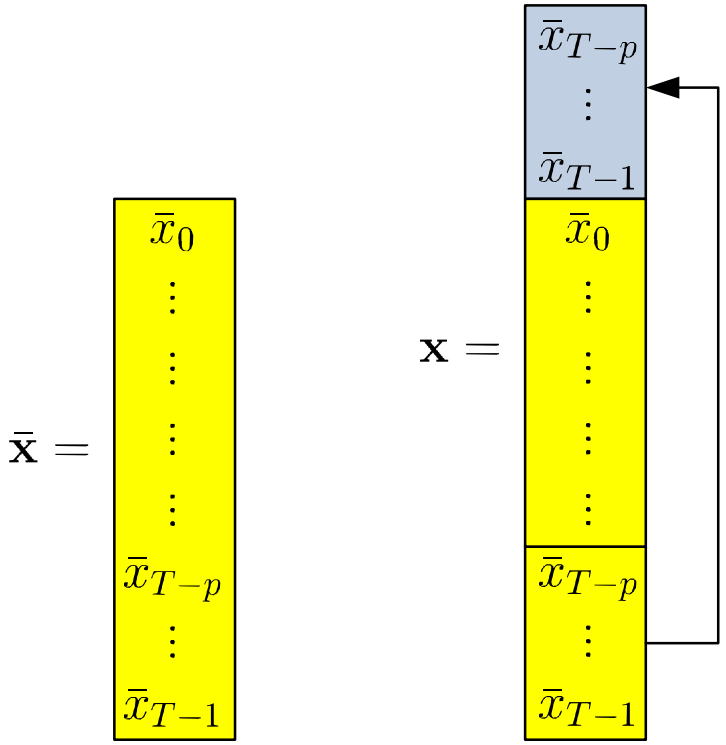
$$\underbrace{\begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_p \\ \vdots \\ \vdots \\ y_{T-1} \end{bmatrix}}_{=\mathbf{y}} \approx \underbrace{\begin{bmatrix} h_0 & & & & h_p & \dots & h_1 \\ h_1 & h_0 & & & & \ddots & \vdots \\ \vdots & & \ddots & & & & h_p \\ h_p & \dots & h_1 & h_0 & & & \\ & \ddots & & & \ddots & & \\ & & \ddots & & & \ddots & \\ & & & h_p & \dots & h_1 & h_0 \end{bmatrix}}_{=\mathbf{A}\in\mathbb{R}^{T\times T}} \underbrace{\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_p \\ \vdots \\ \vdots \\ x_{T-1} \end{bmatrix}}_{=\mathbf{x}} + \underbrace{\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_p \\ \vdots \\ \vdots \\ v_{T-1} \end{bmatrix}}_{=\mathbf{v}}$$

  - appears to be a reasonable approximation if $p \ll T$
    - a common trick in image processing problems such as deblurring (2D)
  - in communications we can even make circulant systems happen

OFDM in Communications

- let $\{\bar{x}_t\}_{t=0}^{T-1}$ be the input signal block we want to send
- *physically* transmit the input signal block $\{x_t\}_{t=0}^{T+p-1}$ this way:

$$x_t = \bar{x}_{t+T-p}, \quad t = 0, 1, \ldots, p-1; \qquad x_{t+p} = \bar{x}_t, \quad t = 0, 1, \ldots, T-1$$



OFDM in Communications

- ignore $\{y_t\}_{t=0}^{p-1}$ and consider $\{y_t\}_{t=p}^{T+p-1}$ only. It can be verified that

$$\underbrace{\begin{bmatrix} y_p \\ y_{p+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ y_{T+p-1} \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} h_0 & & & & h_p & \dots & h_1 \\ h_1 & h_0 & & & & \ddots & \vdots \\ \vdots & & \ddots & & & & h_p \\ h_p & \dots & h_1 & h_0 & & & \\ & \ddots & & & \ddots & & \\ & & \ddots & & & \ddots & \\ & & & h_p & \dots & h_1 & h_0 \end{bmatrix}}_{=\mathbf{A}} \underbrace{\begin{bmatrix} \bar{x}_0 \\ \bar{x}_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \bar{x}_{T-1} \end{bmatrix}}_{\bar{\mathbf{x}}} + \underbrace{\begin{bmatrix} v_p \\ v_{p+1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ v_{T+p-1} \end{bmatrix}}_{=\mathbf{v}}$$

- transceiver scheme 1:
  - transmitter side: put info. in $\bar{\mathbf{x}}$; e.g., $\bar{\mathbf{x}} \in \{-1, 1\}^T$ for binary signaling
  - receiver side: estimate $\bar{\mathbf{x}}$ by solving $\mathbf{y} = \mathbf{A}\bar{\mathbf{x}}$ for circulant $\mathbf{A}$; 1 FFT$+$ 1 IFFT
  - such a transceiver scheme is called single-carrier modulation (SCM)

OFDM in Communications

- recall

$$\mathbf{y} = \mathbf{A}\bar{\mathbf{x}} + \mathbf{v} = \mathbf{\Phi}\mathbf{D}\mathbf{\Phi}^H\bar{\mathbf{x}} + \mathbf{v}$$

- transceiver scheme 2:
  - transmitter side: $\bar{\mathbf{x}} = \mathbf{\Phi}\tilde{\mathbf{x}}$ where $\tilde{\mathbf{x}}$ is the info. signal block (say, $\tilde{\mathbf{x}} \in \{-1, 1\}^T$ for binary signaling); 1 IFFT
  - receiver side: $\mathbf{y} = \mathbf{\Phi}\mathbf{D}\tilde{\mathbf{x}} + \mathbf{v}$, so estimate $\tilde{\mathbf{x}}$ via $\mathbf{D}^{-1}\mathbf{\Phi}^H\mathbf{y}$; 1 FFT
  - such a transceiver scheme is called orthogonal frequency division multiplexing (OFDM)

- further reading: OFDM details such as cyclic prefix insertion and removal, noise amplification effects, comparison of OFDM and SCM, MMSE receiver; they have been widely described in the literature, so find literature by yourself

Localization

- Aim: locate the Cartesian coordinate of a sensor or device using distance info.

  – applications: localization in a wireless sensor network, GPS

- let $\mathbf{x} \in \mathbb{R}^2$ be the coordinate of the sensor

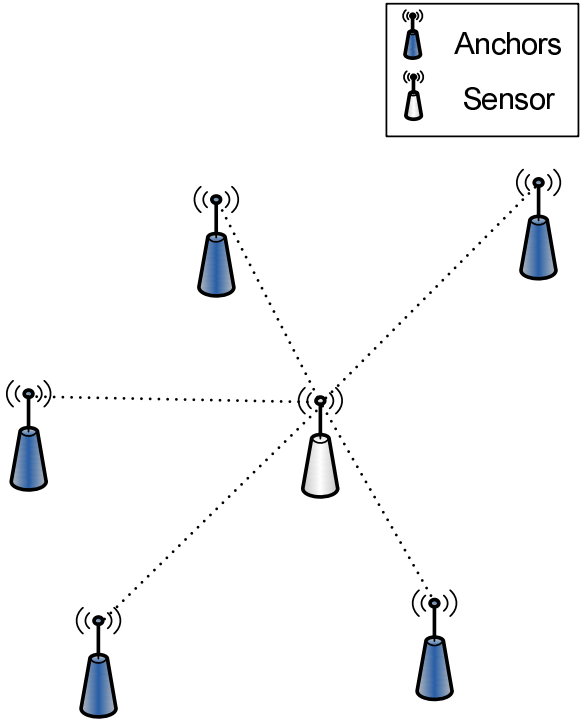
- the sensor communicates with anchors, which are sensors or devices that know their locations

- let $\mathbf{a}_i \in \mathbb{R}^2$, $i = 1, \ldots, m$, be the anchors' locations

- the sensor measures the distances

$$d_i = \|\mathbf{x} - \mathbf{a}_i\|_2, \ i = 1, \ldots, m,$$

  which can be done by time-of-arrival measurements, received signal strength measurements, ping-pong,...



Localization

- observe that

$$d_i^2 = \|\mathbf{x} - \mathbf{a}_i\|_2^2 = \|\mathbf{x}\|_2^2 - 2\mathbf{a}_i^T\mathbf{x} + \|\mathbf{a}_i\|_2^2, \quad i = 1, \ldots, m,$$

and re-organize the equations as a matrix equation

$$\begin{bmatrix} \|\mathbf{a}_1\|_2^2 - d_1^2 \\ \vdots \\ \|\mathbf{a}_m\|_2^2 - d_m^2 \end{bmatrix} = \begin{bmatrix} 2\mathbf{a}_1^T & -1 \\ \vdots & \vdots \\ 2\mathbf{a}_m^T & -1 \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \|\mathbf{x}\|_2^2 \end{bmatrix}.$$

Note that the above matrix equation is nonlinear.

- Idea: solve the linear matrix equation

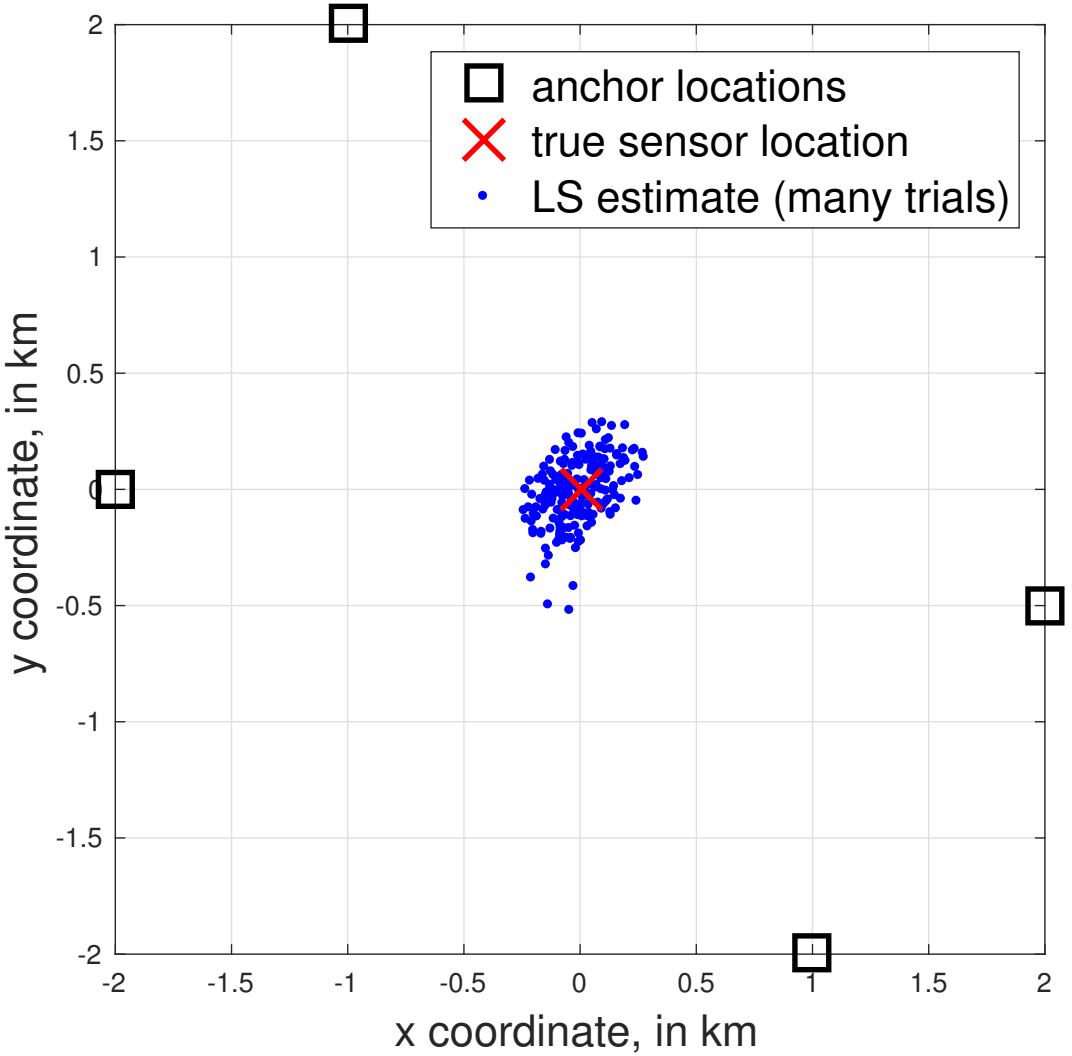
$$\underbrace{\begin{bmatrix} \|\mathbf{a}_1\|_2^2 - d_1^2 \\ \vdots \\ \|\mathbf{a}_m\|_2^2 - d_m^2 \end{bmatrix}}_{=\mathbf{y}} = \underbrace{\begin{bmatrix} 2\mathbf{a}_1^T & -1 \\ \vdots & \vdots \\ 2\mathbf{a}_m^T & -1 \end{bmatrix}}_{=\mathbf{A}} \begin{bmatrix} \mathbf{x} \\ z \end{bmatrix}$$

where $(\mathbf{x}, z)$ is a *free variable* on $\mathbb{R}^3$; or, no constraint $z = \|\mathbf{x}\|_2^2$

Localization

- in practice, the sensor obtains noisy measurements $\hat{d}_i = d_i + v_i,\ i = 1, \ldots, m$, where v_t is noise
- we do the engineers' way:
  - replace d_i's by $\hat{d}_i$'s, and compute the LS solution $\mathbf{u} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$;
  - use $\hat{\mathbf{x}} = [\ u_1, u_2\ ]^T$ as the location estimate
- further reading: **[Sayed-Tarighat-Khajehnouri'05]**

Localization Demo.



Number of anchors: $m = 4$. Noise standard deviation: 0.1581km. Number of trials: 200.

Part II: Least Squares

LS Solution

Theorem 2.1. A vector $\mathbf{x}_{\text{LS}}$ is an optimal solution to the LS problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \ \|\mathbf{y}-\mathbf{A}\mathbf{x}\|_2^2$$

if and only if it satisfies

$$\mathbf{A}^T\mathbf{A}\mathbf{x}_{\text{LS}} = \mathbf{A}^T\mathbf{y}. \qquad (*)$$

- the optimality condition in $(*)$ is true for any $\mathbf{A}$, not just full-column rank $\mathbf{A}$
- suppose that $\mathbf{A}$ has full-column rank
  - $\mathbf{A}^T\mathbf{A}$ is nonsingular (verify as a mini-exercise)
  - the solution to $(*)$ is uniquely given by $\mathbf{x}_{\text{LS}} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$
- $(*)$ is called the normal equations
- the same result holds for the complex case, viz., $\mathbf{A}^H\mathbf{A}\mathbf{x}_{\text{LS}} = \mathbf{A}^H\mathbf{y}$

LS and the Projection Theorem

- Theorem 2.1 can be shown using the projection theorem
- let $\mathbf{x}_{\text{LS}}$ be an LS solution, and observe that

$$\Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \arg \min_{\mathbf{z} \in \mathcal{R}(\mathbf{A})} \|\mathbf{z} - \mathbf{y}\|_2^2 = \mathbf{A}\mathbf{x}_{\text{LS}}$$

- by the projection theorem (Theorem 1.2 in Lecture 1), we have

$$\begin{aligned} \Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \mathbf{A}\mathbf{x}_{\text{LS}} \quad &\Longleftrightarrow \quad \mathbf{z}^T(\mathbf{A}\mathbf{x}_{\text{LS}} - \mathbf{y}) = 0 \text{ for all } \mathbf{z} \in \mathcal{R}(\mathbf{A}) \\ &\Longleftrightarrow \quad \mathbf{x}^T\mathbf{A}^T(\mathbf{A}\mathbf{x}_{\text{LS}} - \mathbf{y}) = 0 \text{ for all } \mathbf{x} \in \mathbb{R}^n \\ &\Longleftrightarrow \quad \mathbf{A}^T(\mathbf{A}\mathbf{x}_{\text{LS}} - \mathbf{y}) = 0 \end{aligned}$$

Orthogonal Projections

- the projections of $\mathbf{y}$ onto $\mathcal{R}(\mathbf{A})$ and $\mathcal{R}(\mathbf{A})^\perp$ are, resp.,

$$\Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \mathbf{A}\mathbf{x}_{\text{LS}} = \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$$
$$\Pi_{\mathcal{R}(\mathbf{A})^\perp}(\mathbf{y}) = \mathbf{y} - \Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = (\mathbf{I} - \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T)\mathbf{y}$$

- the orthogonal projector of $\mathbf{A}$ is defined as

$$\mathbf{P}_\mathbf{A} = \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$$

  the orthogonal complement projector of $\mathbf{A}$ is defined as

$$\mathbf{P}_\mathbf{A}^\perp = \mathbf{I} - \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T.$$

- obviously, we want to write $\Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \mathbf{P}_\mathbf{A}\mathbf{y}$, $\Pi_{\mathcal{R}(\mathbf{A})^\perp}(\mathbf{y}) = \mathbf{P}_\mathbf{A}^\perp\mathbf{y}$
- note: a more general definition for orthogonal projectors will be studied later

Orthogonal Projections

- properties of $\mathbf{P_A}$ (same properties apply to $\mathbf{P_A^\perp}$):
  - $\mathbf{P_A}$ is *idempotent*; i.e., $\mathbf{P_A P_A} = \mathbf{P_A}$
  - $\mathbf{P_A} = \mathbf{P_A}^T$
- additional properties that will be revealed in later lectures:
  - the eigenvalues of $\mathbf{P_A}$ are either zero or one
  - $\mathbf{P_A}$ can be written as $\mathbf{P_A} = \mathbf{U}_1\mathbf{U}_1^T$ for some semi-orthogonal $\mathbf{U}_1$
    - we can also prove it here:
      - there always exists a semi-orthogonal $\mathbf{U}_1$ such that $\mathcal{R}(\mathbf{A}) = \mathcal{R}(\mathbf{U}_1)$
      - $\Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \Pi_{\mathcal{R}(\mathbf{U}_1)}(\mathbf{y}) = \mathbf{U}_1\mathbf{U}_1^T\mathbf{y}$
      - as $\Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \Pi_{\mathcal{R}(\mathbf{U}_1)}(\mathbf{y})$ holds for any $\mathbf{y}$, or $(\mathbf{P_A} - \mathbf{U}_1\mathbf{U}_1^T)\mathbf{y} = \mathbf{0}$ for any $\mathbf{y}$, we must have $\mathbf{P_A} = \mathbf{U}_1\mathbf{U}_1^T$

Pseudo-Inverse

- the pseudo-inverse of a full-column-rank $\mathbf{A}$ is defined as

$$\mathbf{A}^\dagger = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T.$$

- $\mathbf{A}^\dagger$ satisfies $\mathbf{A}^\dagger\mathbf{A} = \mathbf{I}$, but not necessarily $\mathbf{A}\mathbf{A}^\dagger = \mathbf{I}$
- $\mathbf{A}^\dagger\mathbf{y}$ is the LS solution
- note: a more general definition for the pseudo-inverse will be studied later

LS by Convex Optimization

- we can also prove the LS optimality condition by optimization
- the gradient of a continuously differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is defined as

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

- Fact: consider an unconstrained optimization problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} \; f(\mathbf{x})$$

  where $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable

  - suppose f is convex (we skip the def. here). A point $\mathbf{x}^\star$ is an optimal solution if and only if $\nabla f(\mathbf{x}^\star) = \mathbf{0}$
  - for non-convex f, any point $\hat{\mathbf{x}}$ satisfying $\nabla f(\hat{\mathbf{x}}) = \mathbf{0}$ is a stationary point

LS by Convex Optimization

- Fact: consider a quadratic function

$$f(\mathbf{x}) = \tfrac{1}{2}\mathbf{x}^T\mathbf{R}\mathbf{x} + \mathbf{q}^T\mathbf{x} + c,$$

  where $\mathbf{R} \in \mathbb{R}^{n\times n}$ is symmetric; i.e., $r_{ij} = r_{ji}$ for all i, j.

  - $\nabla f(\mathbf{x}) = \mathbf{R}\mathbf{x} + \mathbf{q}$
  - f is convex if $\mathbf{R}$ is positive semidefinite (PSD); for now it suffices to know that if $\mathbf{R}$ takes the form $\mathbf{R} = \mathbf{A}^T\mathbf{A}$ for some $\mathbf{A}$, it is PSD

- the LS objective function is

$$f(\mathbf{x}) = \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_2^2 = \mathbf{x}^T\mathbf{A}^T\mathbf{A}\mathbf{x} - 2(\mathbf{A}^T\mathbf{y})^T\mathbf{x} + \|\mathbf{y}\|_2^2.$$

  Using the above optimization facts, $\mathbf{x}_{\text{LS}}$ is an LS optimal solution if and only if $\mathbf{A}^T\mathbf{A}\mathbf{x}_{\text{LS}} - \mathbf{A}^T\mathbf{y} = \mathbf{0}$.

LS by Convex Optimization

- using optimization results is handy in some (actually, many) cases
- example: consider a regularized LS problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \ \|\mathbf{y}-\mathbf{A}\mathbf{x}\|_2^2+\lambda\|\mathbf{x}\|_2^2, \qquad \text{for some constant } \lambda>0.$$

  - solution by optimization: $\nabla f(\mathbf{x})=2\mathbf{A}^T\mathbf{A}\mathbf{x}-2\mathbf{A}^T\mathbf{y}+2\lambda\mathbf{x}$. Thus the optimal solution is

$$\mathbf{x}_{\text{RLS}}=(\mathbf{A}^T\mathbf{A}+\lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{y}$$

  - solution by the projection thm., in contrast: have to rewrite the problem as

$$\min_{\mathbf{x}\in\mathbb{R}^n} \ \left\|\begin{bmatrix}\mathbf{y}\\ \mathbf{0}\end{bmatrix}-\begin{bmatrix}\mathbf{A}\\ \sqrt{\lambda}\mathbf{I}\end{bmatrix}\mathbf{x}\right\|_2^2,$$

    and use the projection theorem to get the same result.

Part III-A: Matrix Factorization

Matrix Factorization

There are also many applications in which we deal with a representation of multiple given $\mathbf{y}_i$'s via

$$\mathbf{y}_i = \mathbf{A}\mathbf{b}_i + \mathbf{v}_i, \quad i = 1, \ldots, n,$$

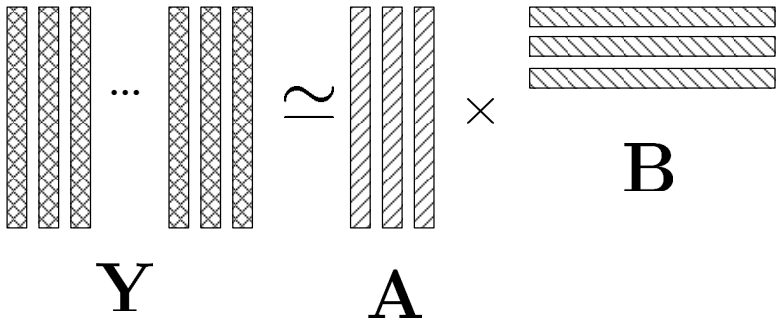
where $\mathbf{A} \in \mathbb{R}^{n \times k}$, $\mathbf{b}_i \in \mathbb{R}^k$, $i = 1, \ldots, n$; $\mathbf{v}_i$'s are noise. In particular, both $\mathbf{b}_i$'s and $\mathbf{A}$ are to be determined.

- for example, in basis representation, we want to learn the dictionary from data

Matrix Factorization

Problem: given $\mathbf{Y} \in \mathbb{R}^{m \times n}$ and a positive integer $k < \min\{m, n\}$, solve

$$\min_{\mathbf{A} \in \mathbb{R}^{m \times k}, \mathbf{B} \in \mathbb{R}^{k \times n}} \|\mathbf{Y} - \mathbf{AB}\|_F^2$$



- also called low-rank matrix approximation: let $\mathbf{Z} = \mathbf{AB}$. It has $\text{rank}(\mathbf{Z}) \leq k$.

Principal Component Analysis

Aim: given a collection of data points $\mathbf{y}_1, \ldots, \mathbf{y}_n \in \mathbb{R}^m$, perform a low-dimensional representation

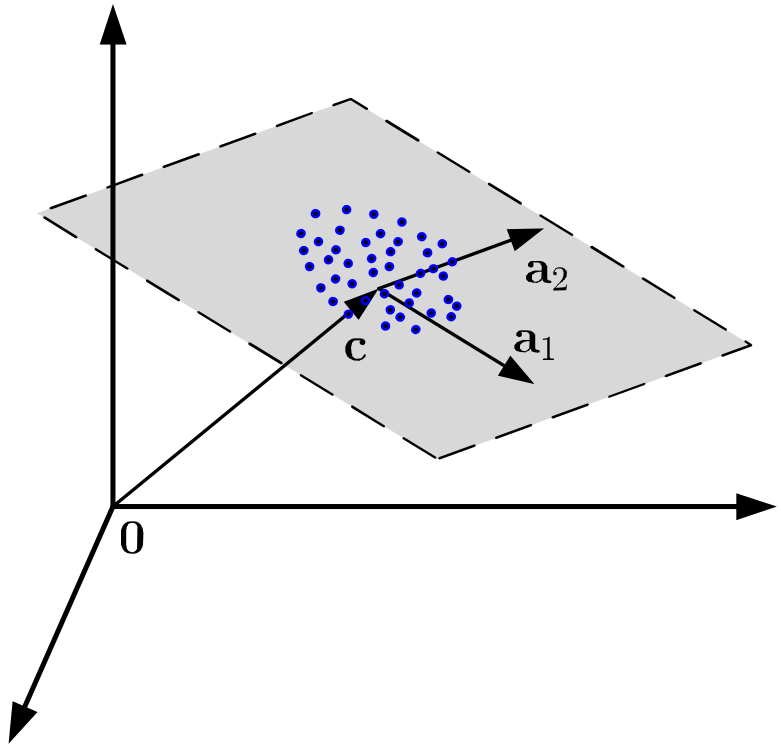
$$\mathbf{y}_i = \mathbf{A}\mathbf{b}_i + \mathbf{c} + \mathbf{v}_i, \quad i = 1, \ldots, n,$$

where $\mathbf{A} \in \mathbb{R}^{m \times k}$ is a basis matrix; $\mathbf{b}_i \in \mathbb{R}^k$ is the coefficient for $\mathbf{y}_i$; $\mathbf{c} \in \mathbb{R}^m$ is the base or mean in statistics terms; $\mathbf{v}_i$ is noise or modeling error.

- Principal component analysis (PCA):
  - choose $\mathbf{c} = \frac{1}{n}\sum_{i=1}^n \mathbf{y}_i$
  - let $\bar{\mathbf{y}}_i = \mathbf{y}_i - \mathbf{c}$, and solve

$$\min_{\mathbf{A},\mathbf{B}} \ \|\bar{\mathbf{Y}} - \mathbf{A}\mathbf{B}\|_F^2$$

  - we may also want a semi-orthogonal $\mathbf{A}$



Principal Component Analysis

- applications: dimensionality reduction, visualization of high-dimensional data, compression, extraction of meaningful features from data,...

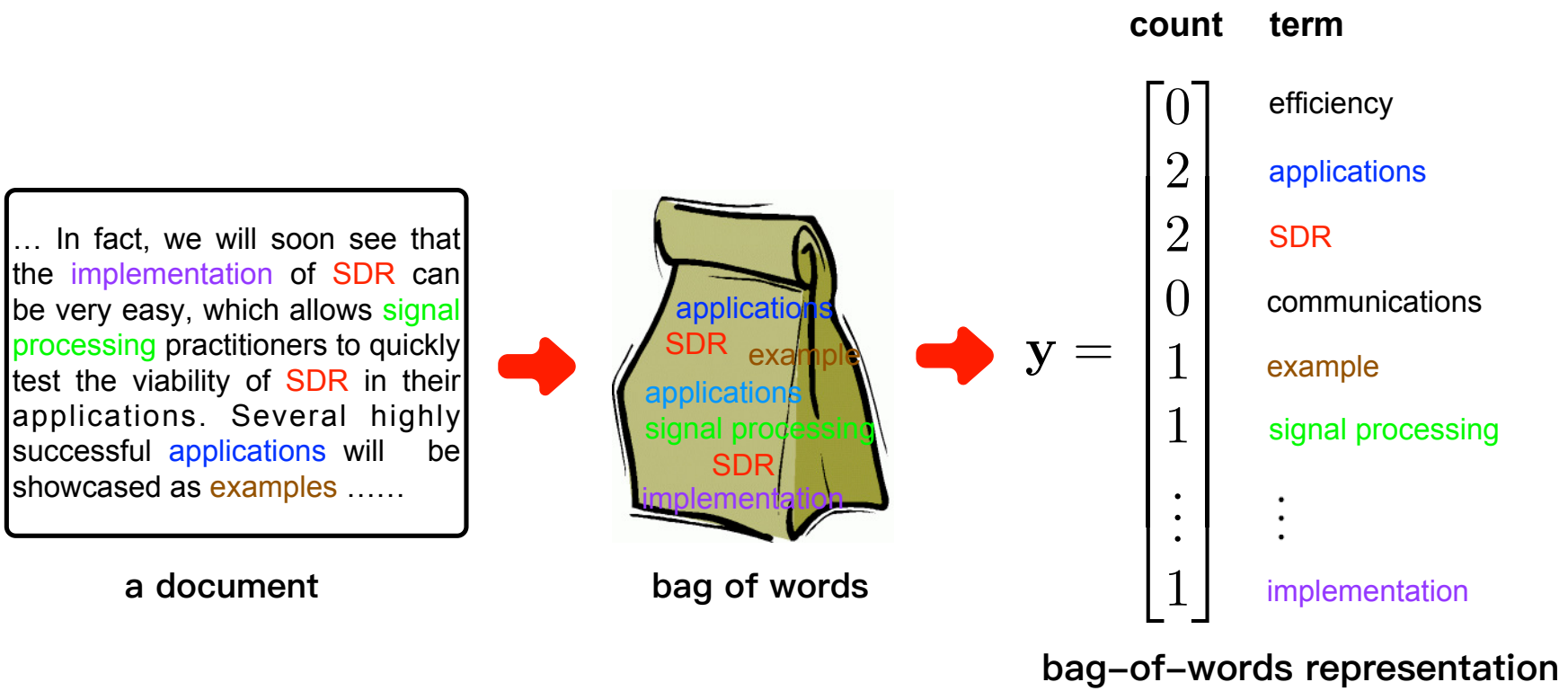
- an example:

  – senate voting: http://livebooklabs.com/keeppies/c5a5868ce26b8125

Topic Modeling

Aim: discover thematic information, or topics, from a (often large) collection of documents, such as books, articles, news, blogs,...

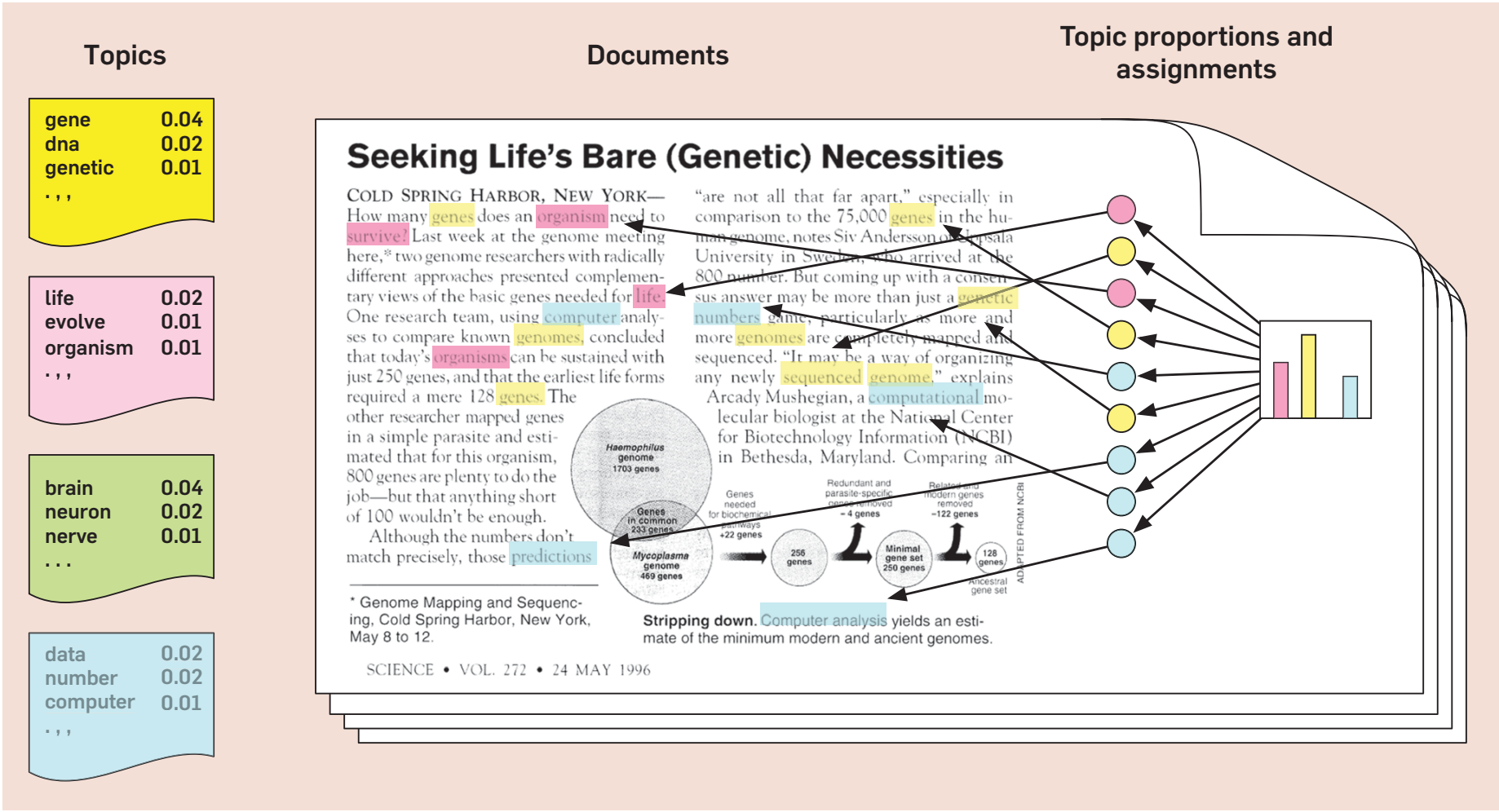
- bag-of-words representation: represent each document as a vector of word counts



Topic Modeling

- let n be the number of documents
- let $\mathbf{y}_i \in \mathbb{R}^m$ be the bag-of-words representation of the ith document, $i = 1, \ldots, n$
- let $\mathbf{Y} = [\ \mathbf{y}_1, \ldots \mathbf{y}_n\ ] \in \mathbb{R}^{m \times n}$, called the term-document matrix
- hypotheses: **[Turney-Pantel'10]**
  - if documents have similar columns vectors in $\mathbf{Y}$, or similar usage of words, they tend to have similar meanings
  - the topic of a document will probabilistically influence the author's choice of words when writing the document

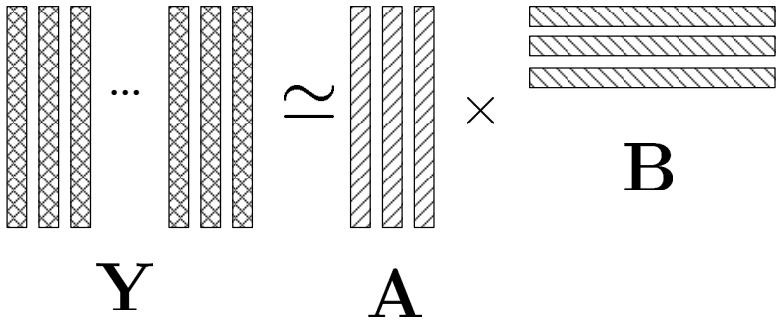
Topic Modeling



Source: **[Blei'12]**.

Topic Modeling

- Problem: apply matrix factorization to a term-document matrix $\mathbf{Y}$

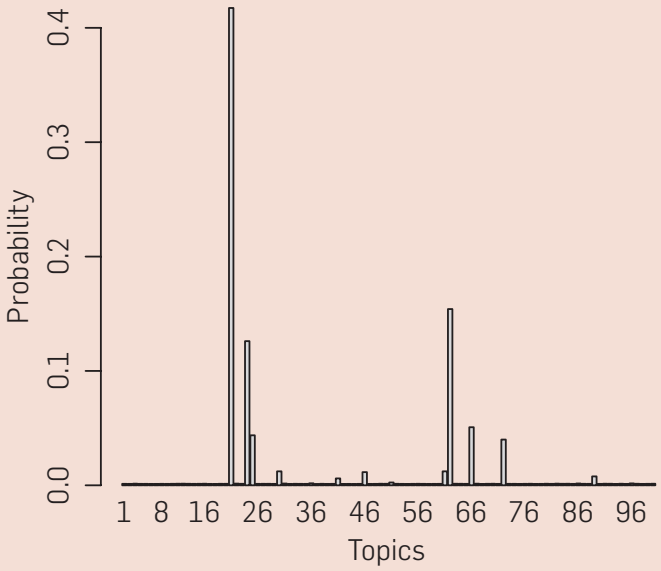


  - $\mathbf{A}$ is called a term-topic matrix, $\mathbf{B}$ is called a topic-document matrix

- Interpretation:

  - each column $\mathbf{a}_i$ of $\mathbf{A}$ should represent a theme topic, e.g., local affairs, foreign affairs, politics, sports... in a collection of newspapers
  - as $\mathbf{y}_i \approx \mathbf{A}\mathbf{b}_i$, each document is postulated as a linear combination of topics
  - matrix factorization aims at discovering topics from the documents

Topic Modeling



"Genetics"	"Evolution"	"Disease"	"Computers"
human	evolution	disease	computer
genome	evolutionary	host	models
dna	species	bacteria	information
genetic	organisms	diseases	data
genes	life	resistance	computers
sequence	origin	bacterial	system
gene	biology	new	network
molecular	groups	strains	systems
sequencing	phylogenetic	control	model
map	living	infectious	parallel
information	diversity	malaria	methods
genetics	group	parasite	networks
mapping	new	parasites	software
project	two	united	new
sequences	common	tuberculosis	simulations

Topics found in a real set of documents. Source: **[Blei'12]**. The document set consists of $17,000$ articles from the journal *Science*. The topics are discovered using a technique called *latent Dirichlet allocation*, which is not the same as, but has strong connections to, matrix factorization.

Topic Modeling

- topic modeling via matrix factorization has been used in, or is tightly connected to
  - information retrieval, natural language processing, machine learning
  - document clustering, classification and retrieval
  - latent semantic analysis, latent semantic indexing: finding similarities of documents, finding similarities of terms (are "cars," "Lamborghini," and "Ferrari" related?)

- though not considered in this course, it seems better to also model $\mathbf{A}$, $\mathbf{B}$ as element-wise non-negative—this will lead to *non-negative matrix factorization*

- further reading: **[Turney-Pantel'10]**
  - as an aside, it mentions a related application where computers can achieve a score of 92.5% on multiple-choice synonym questions from TOEFL, whereas the average human score is 64.5%

Matrix Factorization

The matrix factorization problem

$$\min_{\mathbf{A}\in\mathbb{R}^{m\times k},\mathbf{B}\in\mathbb{R}^{k\times n}} \|\mathbf{Y}-\mathbf{AB}\|_F^2$$

- has non-unique factors
  - suppose $(\mathbf{A}^\star,\mathbf{B}^\star)$ is an optimal solution to the problem, and let $\mathbf{Q}\in\mathbb{R}^{k\times k}$ be any nonsingular matrix. Then $(\mathbf{A}^\star\mathbf{Q}^{-1},\mathbf{Q}\mathbf{B}^\star)$ is also an optimal solution.
  - the non-uniqueness of $(\mathbf{A},\mathbf{B})$ makes the above matrix factorization formulation a bad formulation for problems such as topic modeling
- is non-convex, but can be solved by singular value decomposition (beautifully)
- can also be handled by LS

Matrix Factorization

- Alternating LS (ALS): given a starting point $(\mathbf{A}^{(0)}, \mathbf{B}^{(0)})$, do

$$\mathbf{A}^{(i+1)} = \arg \min_{\mathbf{A} \in \mathbb{R}^{m \times k}} \|\mathbf{Y} - \mathbf{A}\mathbf{B}^{(i)}\|_F^2$$

$$\mathbf{B}^{(i+1)} = \arg \min_{\mathbf{B} \in \mathbb{R}^{k \times n}} \|\mathbf{Y} - \mathbf{A}^{(i+1)}\mathbf{B}\|_F^2$$

  for $i = 0, 1, 2, \ldots$, and stop when a stopping rule is satisfied.

- let's make a mild assumption that $\mathbf{A}^{(i)}, \mathbf{B}^{(i)}$ have full rank at every i. Then,

$$\mathbf{A}^{(i+1)} = \mathbf{Y}(\mathbf{B}^{(i)})^T(\mathbf{B}^{(i)}(\mathbf{B}^{(i)})^T)^{-1}, \quad \mathbf{B}^{(i+1)} = ((\mathbf{A}^{(i+1)})^T\mathbf{A}^{(i+1)})^{-1}(\mathbf{A}^{(i+1)})^T\mathbf{Y}$$

- ALS is guaranteed to converge an optimal solution to $\min_{\mathbf{A},\mathbf{B}} \|\mathbf{Y} - \mathbf{A}\mathbf{B}\|_F^2$ under some mild assumptions **[Udell-Horn-Zadeh-Boyd'16]**
  - note: this result is specific and does not directly carry forward to other related problems such as low-rank matrix completion

Low-Rank Matrix Completion

- let $\mathbf{Y} \in \mathbb{R}^{m \times n}$ be a matrix with missing entries, i.e., the values y_{ij}'s are known only for $(i,j) \in \Omega$ where Ω is an index set that indicates the available entries
- Aim: recover the missing entries of $\mathbf{Y}$
- application: recommender system, data science
- example: movie recommendation (further reading: **[Koren-Bell-Volinsky'09]**)
  - $\mathbf{Y}$ records how user i likes movie j
  - $\mathbf{Y}$ has lots of missing entries; a user doesn't watch all movies
  - $\mathbf{Y}$ may be assumed to have low rank; research shows that only a few factors affect users' preferences.

movies

$$\mathbf{Y} = \begin{bmatrix} 2 & 3 & 1 & ? & ? & 5 & 5 \\ 1 & ? & 4 & 2 & ? & ? & ? \\ ? & 3 & 1 & ? & 2 & 2 & 2 \\ ? & ? & ? & 3 & ? & 1 & 5 \end{bmatrix} \text{ users}$$

Low-Rank Matrix Completion

- Problem: given $\{y_{ij}\}_{(i,j)\in\Omega}$, Ω and a positive integer k, solve

$$\min_{\mathbf{A}\in\mathbb{R}^{m\times k},\mathbf{B}\in\mathbb{R}^{k\times n}} \sum_{(i,j)\in\Omega} |y_{ij} - [\mathbf{AB}]_{ij}|^2$$

- ALS can be applied; more tedious to write out the LS solutions than the previous matrix factorization problem but not any harder in principle

- supposingly a very difficult problem, but

- methods like ALS were found to work by means of empirical studies

- recent theoretical research suggests that matrix completion may not be that hard under some assumptions, e.g., ALS can give good results **[Sun-Luo'16]**

Low-Rank Matrix Completion

- an ALS alternative to matrix completion (easier to program):
  - consider an equivalent reformulation of the matrix completion problem

$$\min_{\mathbf{A}\in\mathbb{R}^{m\times k},\mathbf{B}\in\mathbb{R}^{k\times n},\mathbf{R}\in\mathbb{R}^{m\times n}} \|\mathbf{Y}-\mathbf{A}\mathbf{B}-\mathbf{R}\|_F^2 \quad \text{s.t. } r_{ij}=0,\ (i,j)\in\Omega$$

  - do alternating optimization

$$\mathbf{A}^{(i+1)} = \arg\min_{\mathbf{A}\in\mathbb{R}^{m\times k}} \|\mathbf{Y}-\mathbf{A}\mathbf{B}^{(i)}-\mathbf{R}^{(i)}\|_F^2$$

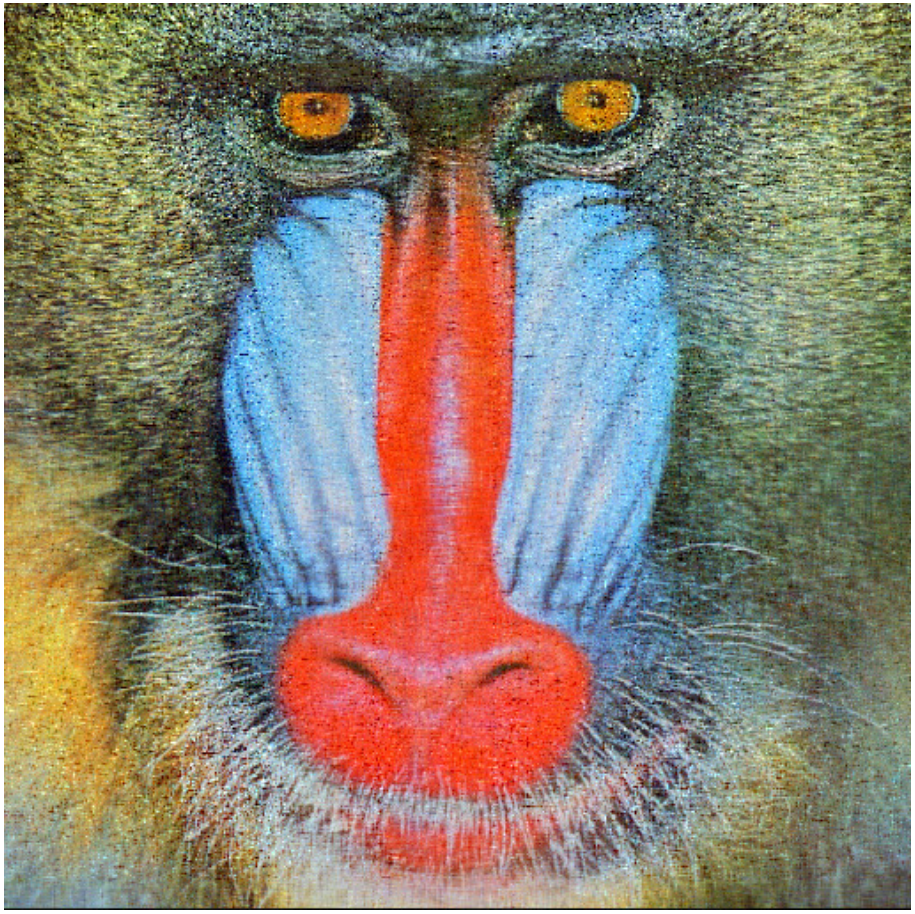
$$\mathbf{B}^{(i+1)} = \arg\min_{\mathbf{B}\in\mathbb{R}^{k\times n}} \|\mathbf{Y}-\mathbf{A}^{(i+1)}\mathbf{B}-\mathbf{R}^{(i)}\|_F^2$$

$$\mathbf{R}^{(i+1)} = \arg\min_{\mathbf{R}\in\mathbb{R}^{m\times n}} \|\mathbf{Y}-\mathbf{A}^{(i+1)}\mathbf{B}^{(i+1)}-\mathbf{R}\|_F^2$$

    the first two are LS as before; the third has a closed form

$$r_{ij}^{(i+1)} = \begin{cases} 0, & (i,j)\in\Omega \\ [\mathbf{Y}-\mathbf{A}^{(i+1)}\mathbf{B}^{(i+1)}]_{i,j}, & (i,j)\notin\Omega \end{cases}$$

Toy Demonstration of Low-Rank Matrix Completion



Left: An incomplete image with 40% missing pixels. Right: the matrix completion result of the algorithm shown on last page. $k = 120$.

Part III-B: Other Extensions

Beyond LS

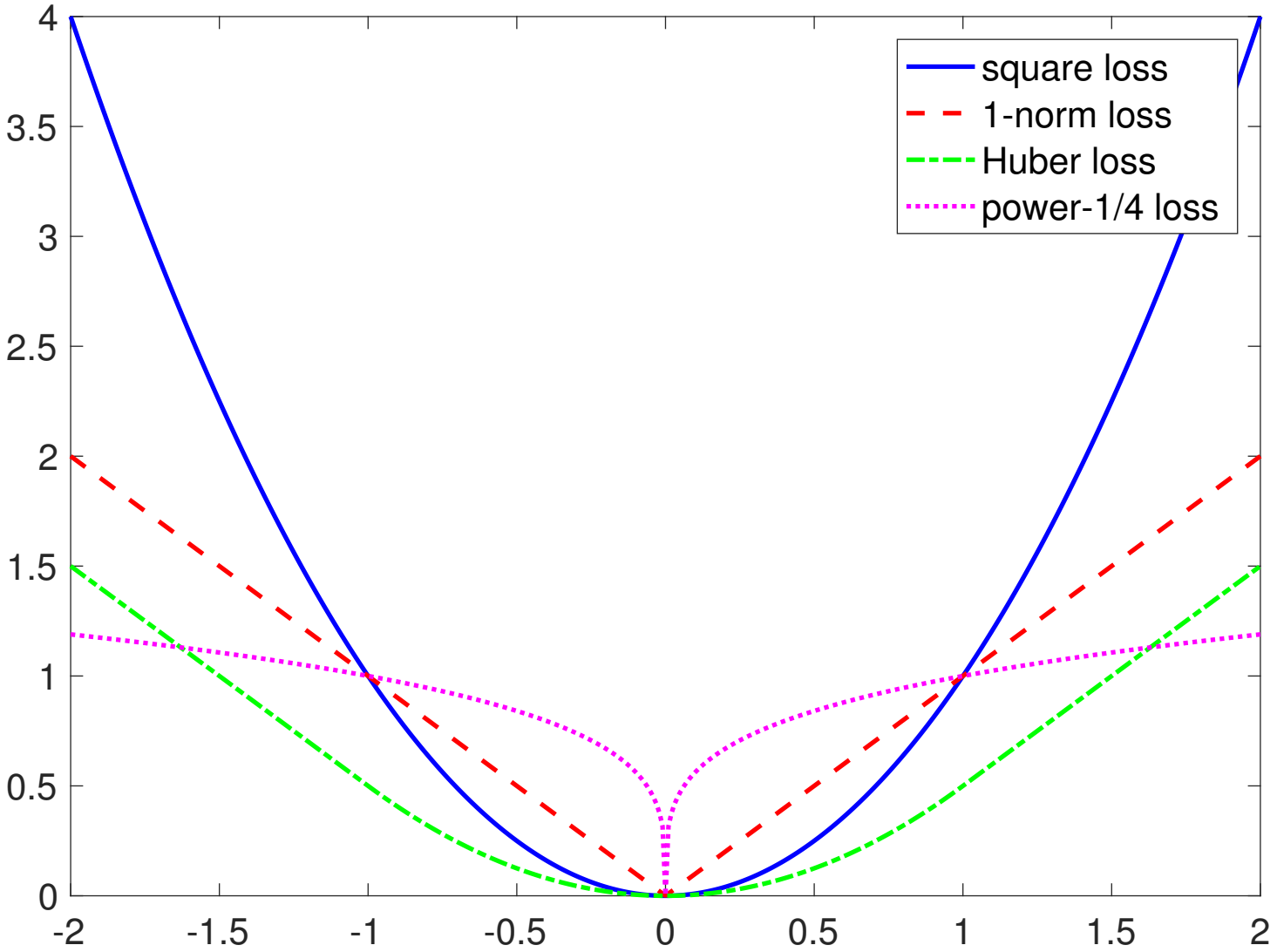
- let $\bar{\mathbf{a}}_i \in \mathbb{R}^n$ denote the ith row of $\mathbf{A}$. The LS problem can be represented as

$$\min_{\mathbf{x}\in\mathbb{R}^n} \sum_{i=1}^{m} \ell(\bar{\mathbf{a}}_i^T\mathbf{x} - y_i)^2$$

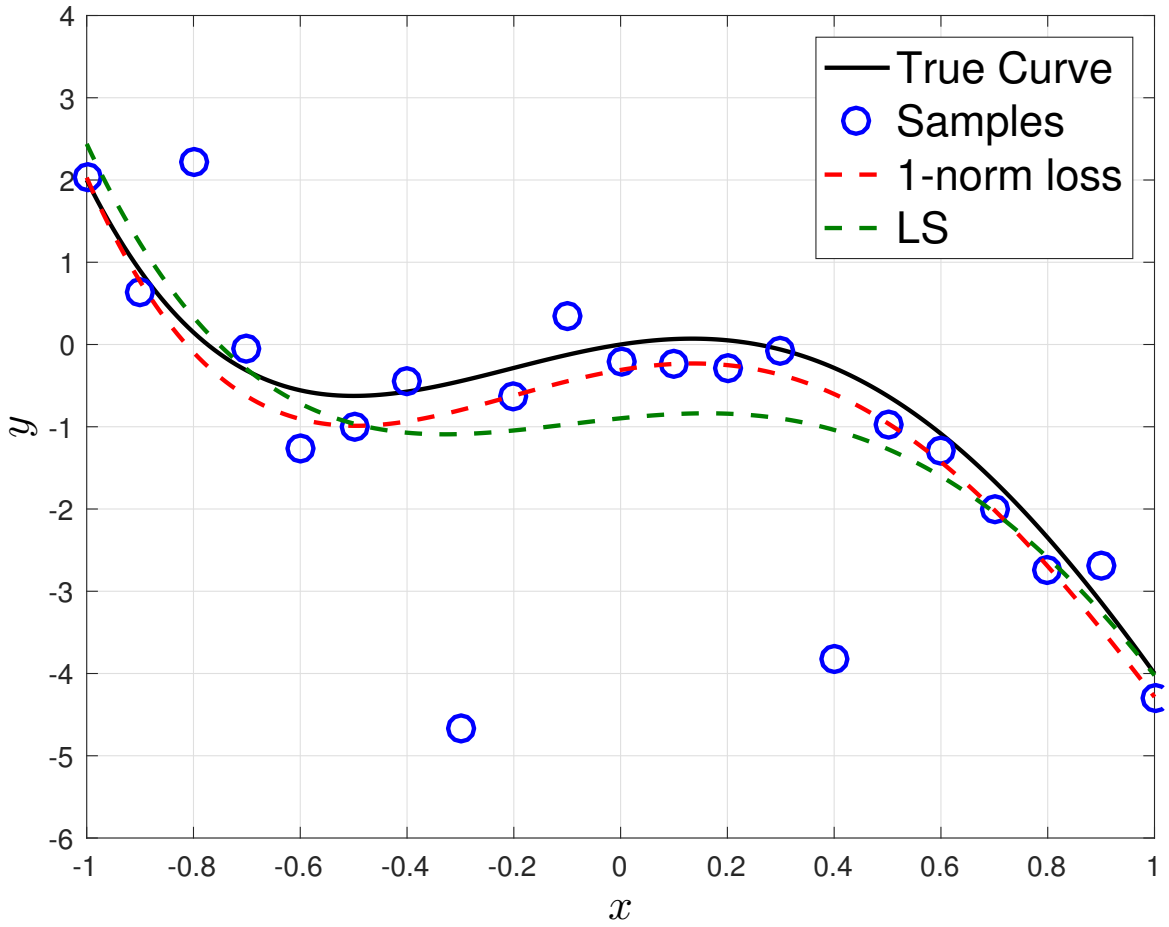
  where $\ell(z) = |z|^2$ denotes the loss function for measuring the badness of fit

- Question: why don't we use other loss functions?
  - we can indeed use other loss functions, such as
    - 1-norm loss: $\ell(z) = |z|$
    - Huber loss: $\ell(z) = \begin{cases} \frac{1}{2}|z|^2, & |z| \le 1 \\ |z| - \frac{1}{2}, & |z| > 1 \end{cases}$
    - power-p loss: $\ell(z) = |z|^p$, with $p < 1$
  - the above loss functions are more robust against outliers, but
  - they require optimization and don't result in a clean closed-form solution as LS

Illustration of Loss Functions



Curve Fitting Example



"True" curve: the true $f(x)$, $p = 5$. The points at $x = -0.3$ and $x = 0.4$ are outliers, and they do not follow the true curve. The 1-norm loss problem is solved by a convex optimization tool.

Gradient Descent

- in LS we need to solve

$$(\mathbf{A}^T\mathbf{A})\mathbf{x}_{\text{LS}} = \mathbf{A}^T\mathbf{y},$$

  and that requires $\mathcal{O}(n^3)$

  – we also need to compute $\mathbf{A}^T\mathbf{A}$ and $\mathbf{A}^T\mathbf{y}$; their complexities are $\mathcal{O}(mn^2)$ and $\mathcal{O}(mn)$, resp.

- $\mathcal{O}(n^3)$ is expensive for very large n

- Question: can we have cheaper LS solutions, perhaps with some compromise of the solution accuracies?

Gradient Descent

- consider a general unconstrained optimization problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \; f(\mathbf{x})$$

  where f is continuously differentiable

- Gradient Descent: given a starting point $\mathbf{x}^{(0)}$, do

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} - \mu \nabla f(\mathbf{x}^{(k-1)}), \quad k = 1, 2, \ldots$$

  where $\mu > 0$ is a step size

- take an optimization course to get more details! It is known that
  - for convex f and under some appropriate choice of μ, gradient descent converges to an optimal solution
  - for non-convex f and under some appropriate choice of μ, gradient descent converges to a stationary point

Gradient Descent

- gradient descent for LS:

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} - 2\mu(\mathbf{A}^T\mathbf{A}\mathbf{x}^{(k-1)} - \mathbf{A}^T\mathbf{y}), \quad k = 0, 1, \ldots$$

- complexity for dense $\mathbf{A}$
  - computing $\mathbf{A}^T\mathbf{A}$ and $\mathbf{A}^T\mathbf{y}$: $\mathcal{O}(mn^2)$ and $\mathcal{O}(mn)$, resp. (same as before)
    - $\mathbf{A}^T\mathbf{A}$ and $\mathbf{A}^T\mathbf{y}$ are cached for subsequent use in gradient descent
  - complexity of each iteration: $\mathcal{O}(n^2)$

- complexity for sparse $\mathbf{A}$
  - computing $\mathbf{A}^T\mathbf{y}$: $\mathcal{O}(\mathrm{nnz}(\mathbf{A}))$
  - complexity of each iteration: $\mathcal{O}(n + \mathrm{nnz}(\mathbf{A}))$
    - $\mathbf{A}^T\mathbf{A}$ is not necessarily sparse, so we do $\mathbf{A}\mathbf{x}^{(k-1)}$ and then $\mathbf{A}^T(\mathbf{A}\mathbf{x}^{(k-1)})$

Gradient Descent

- gradient descent is easy to understand, but there are better algorithms...

- further reading: the conjugate gradient method; see, e.g., https://stanford.edu/class/ee364b/lectures/conj_grad_slides.pdf

Online LS

- recall the LS formulation

$$\min_{\mathbf{x}\in\mathbb{R}^n} \sum_{t=1}^{m} |\bar{\mathbf{a}}_t^T \mathbf{x} - y_t|^2$$

- the LS we learnt is a batch process; i.e., solve one $\mathbf{x}$ given the whole $(\mathbf{A}, \mathbf{y})$

- there are many applications where new $(\bar{\mathbf{a}}_t, y_t)$ appears as time goes, and we want the process to be adaptive or in real time; i.e., $\mathbf{x}$ is updated with t

Incremental Gradient Descent

- consider an optimization problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \sum_{t=1}^{m} f_t(\mathbf{x})$$

  where every f_t is continuously differentiable

- Incremental Gradient Descent:

$$\mathbf{x}_t = \mathbf{x}_{t-1} - \mu \nabla f_t(\mathbf{x}_{t-1}), \quad t = 1, 2, \ldots$$

  – also called stochastic gradient descent, least mean squares (LMS) (in 70's), ...

- incremental gradient descent for LS:

$$\mathbf{x}_t = \mathbf{x}_{t-1} + 2\mu(y_t - \bar{\mathbf{a}}_t^T \mathbf{x}_{t-1})\bar{\mathbf{a}}_t$$

Recursive LS

- Recursive LS (RLS) formulation:

$$\mathbf{x}_t = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \sum_{i=1}^{t} \lambda^{t-i} |\bar{\mathbf{a}}_i^T \mathbf{x} - y_i|^2$$

  where $0 < \lambda \leq 1$ is a prescribed constant and is called the forgetting factor

  - weigh the importance of $|\bar{\mathbf{a}}_i^T \mathbf{x} - y_i|^2$ w.r.t. time t; the present is most important; distant pasts are insignificant; how much we remember the pasts depends on λ

- at first look, the RLS solution is $\mathbf{x}_t = \mathbf{R}_t^{-1}\mathbf{q}_t$, where

$$\mathbf{R}_t = \sum_{i=1}^{t} \lambda^{t-i} \bar{\mathbf{a}}_i \bar{\mathbf{a}}_i^T, \quad \mathbf{q}_t = \sum_{i=1}^{t} \lambda^{t-i} y_i \bar{\mathbf{a}}_i$$

- a recursive formula for $\mathbf{x}_t$ can be derived by using the Woodbury matrix identity and by using the problem structures carefully

Woodbury Matrix Identity

For $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ of appropriate dimensions, we have

$$(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} = \mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{B}(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})^{-1}\mathbf{C}\mathbf{A}^{-1},$$

assuming that the inverses above exist.

- for the RLS problem, it is sufficient to know the special case

$$(\mathbf{A} + \mathbf{b}\mathbf{b}^T)^{-1} = \mathbf{A}^{-1} - \frac{1}{1 + \mathbf{b}^T\mathbf{A}^{-1}\mathbf{b}}\mathbf{A}^{-1}\mathbf{b}\mathbf{b}^T\mathbf{A}^{-1}$$

Recursive LS

- it can be verified that $\mathbf{R}_t = \lambda \mathbf{R}_{t-1} + \bar{\mathbf{a}}_t \bar{\mathbf{a}}_t^T$, $\mathbf{q}_t = \lambda \mathbf{q}_{t-1} + y_t \bar{\mathbf{a}}_t$
- by the Woodbury matrix identity,

$$\mathbf{R}_t^{-1} = (\lambda \mathbf{R}_{t-1} + \bar{\mathbf{a}}_t \bar{\mathbf{a}}_t^T)^{-1} = \tfrac{1}{\lambda}\mathbf{R}_{t-1}^{-1} - \frac{1}{1 + \frac{1}{\lambda}\bar{\mathbf{a}}_t^T \mathbf{R}_{t-1}^{-1} \bar{\mathbf{a}}_t} (\tfrac{1}{\lambda}\mathbf{R}_{t-1}^{-1}\bar{\mathbf{a}}_t)(\tfrac{1}{\lambda}\mathbf{R}_{t-1}^{-1}\bar{\mathbf{a}}_t)^T$$

- let $\mathbf{P}_t = \mathbf{R}_t^{-1}$ and $\mathbf{g}_t = \dfrac{1}{1 + \frac{1}{\lambda}\bar{\mathbf{a}}_t^T \mathbf{R}_{t-1}^{-1} \bar{\mathbf{a}}_t} (\tfrac{1}{\lambda}\mathbf{R}_{t-1}^{-1}\bar{\mathbf{a}}_t)$. We have

$$\mathbf{g}_t = \frac{1}{1 + \frac{1}{\lambda}\bar{\mathbf{a}}_t^T \mathbf{P}_{t-1} \bar{\mathbf{a}}_t} (\tfrac{1}{\lambda}\mathbf{P}_{t-1}\bar{\mathbf{a}}_t)$$

$$\mathbf{P}_t = \tfrac{1}{\lambda}\mathbf{P}_{t-1} - \mathbf{g}_t (\tfrac{1}{\lambda}\mathbf{P}_{t-1}\bar{\mathbf{a}}_t)^T$$

$$\begin{aligned}\mathbf{x}_t = \mathbf{P}_t \mathbf{q}_t &= \mathbf{P}_{t-1}\mathbf{q}_{t-1} - \lambda \mathbf{g}_t (\tfrac{1}{\lambda}\mathbf{P}_{t-1}\bar{\mathbf{a}}_t)^T \mathbf{q}_{t-1} + \tfrac{1}{\lambda} y_t \mathbf{P}_{t-1}\bar{\mathbf{a}}_t - y_t \mathbf{g}_t (\tfrac{1}{\lambda}\mathbf{P}_{t-1}\bar{\mathbf{a}}_t)^T \bar{\mathbf{a}}_t \\ &= \mathbf{x}_{t-1} - (\bar{\mathbf{a}}_t^T \mathbf{x}_{t-1})\mathbf{g}_t + y_t \mathbf{g}_t\end{aligned}$$

Recursive LS

- summary of the RLS recursion:

$$\mathbf{g}_t = \frac{1}{1 + \frac{1}{\lambda}\bar{\mathbf{a}}_t^T \mathbf{P}_{t-1}\bar{\mathbf{a}}_t}\left(\tfrac{1}{\lambda}\mathbf{P}_{t-1}\bar{\mathbf{a}}_t\right)$$

$$\mathbf{P}_t = \tfrac{1}{\lambda}\mathbf{P}_{t-1} - \mathbf{g}_t\left(\tfrac{1}{\lambda}\mathbf{P}_{t-1}\bar{\mathbf{a}}_t\right)^T$$

$$\mathbf{x}_t = \mathbf{x}_{t-1} + (y_t - \bar{\mathbf{a}}_t^T \mathbf{x}_{t-1})\mathbf{g}_t$$

- remarks:
  - comparison with incremental gradient descent: it replaces $\mathbf{g}_t$ with $2\mu\bar{\mathbf{a}}_t$
  - the above RLS recursion may be numerically unstable as empirical results suggested; modified RLS schemes were developed to mend this issue

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