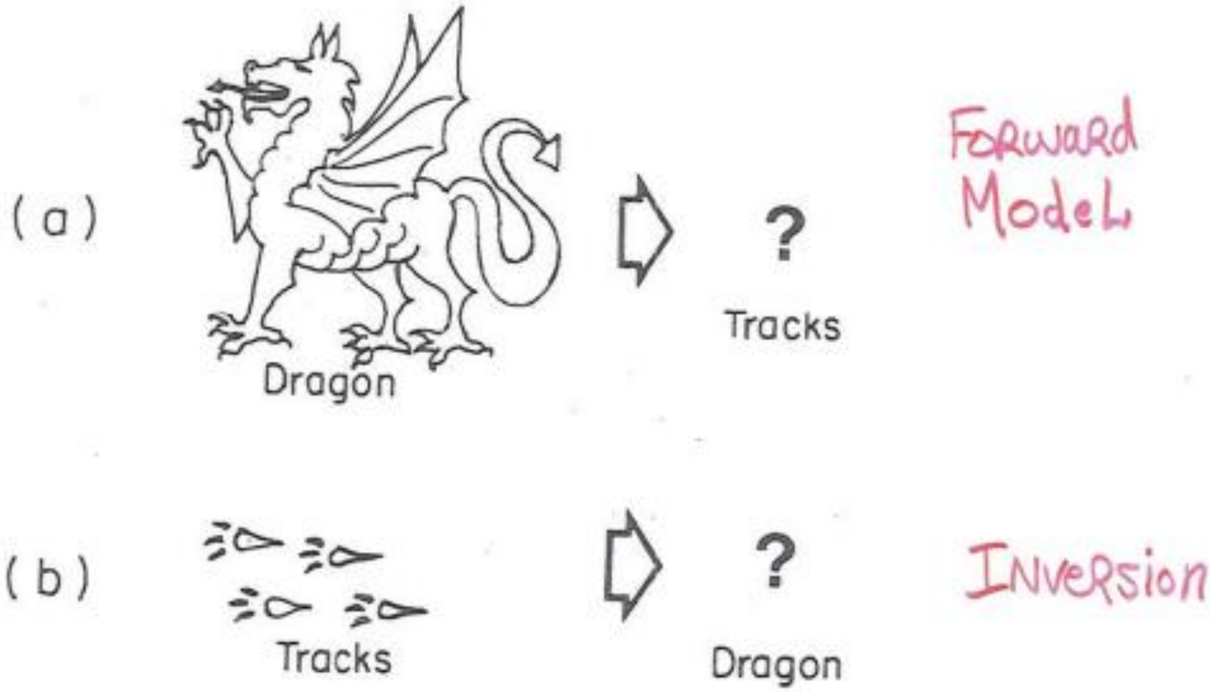
Inversion

How we go from “data” to something useful with lots of slides stolen from Dr. Kane.



Another CHEESEY EXAMPLE

(a) FUN - INVERSE → (386) 468-3773

phone # mnemonic with letters

phone #

(b) (386)468-3773 → ?

phone #

mnemonic

Q: unique soln. ???

Have you done this before?

- Our brains are constantly performing some sort of inversion algorithm
  - Especially hearing
  - How do we locate where something is at?

- We did a simple example:
  - Absorption of dye of light by dye to measure the concentration
  - We looked at mixtures of oil and differentiated the fluorescence spectrum

We’re going from something measured (voltage on an antenna, absorbance, how much light there is, Arrival time) to information (music on the radio, concentration, colors of things, where something is at.

$$g = A\{f\}$$

DATA (NOISY!)

FORWARD* Model

Desired signal or state

* in some cases, may also include "data"...

$\Rightarrow$ $\hat{f}$ = estimate (Retrieval) of f given g ...

w/ $\Gamma_{\hat{f}}$ given Γ_g

error on estimate

(best if kernels/weighting functions of A are orthogonal)

Now, in case of discrete measurements* & retrievals,

A is a matrix $\xrightarrow[\text{Algebra}]{\text{Linear}}$

*or "discretized"

Often useful to do it as a system of linear equations

Here's some simple data

Concentration (µg/mL)	Absorbance
0.000	0.000
0.100	0.006
0.200	0.013
0.300	0.020
0.400	0.023
0.500	0.033
0.600	0.039
0.700	0.046
1.000	0.066

Information we want

What we measured

How do we go from Absorbance to Concentration?

Linear Mappings

$$\vec{\mathbf{g}} = \mathbf{A}\vec{\mathbf{f}}$$

Input (Domain) is vector $\vec{v} \in \mathbb{R}^N$

$\vec{v}$ Relative to $\{\vec{e}_i^{\,N}\}_1^N$ is $(v_1, v_2, \ldots v_N)$

Output (Range) is Vector $\vec{u} \in \mathbb{R}^M$

$\vec{u}$ Relative to $\{\vec{e}_i^{\,M}\}_1^M$ is $(u_1, u_2, \ldots u_M)$

Mapping $A: \mathbb{R}^N \to \mathbb{R}^M$ w/ $\vec{u} = A(\vec{v})$

Now, A is Linear iff:

M is NOT necessarily equal to N

* $A(\alpha \vec{v}) = \alpha A(\vec{v})$
* $A(\vec{v}_1 + \vec{v}_2) = A(\vec{v}_1) + A(\vec{v}_2)$

so, if A is Linear, we have:

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_M \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_N \end{bmatrix}$$

$$\vec{u} = A\vec{v}$$

where A is Represented by a Matrix

Concentration (µg/mL)	Absorbance
0.000	0.000
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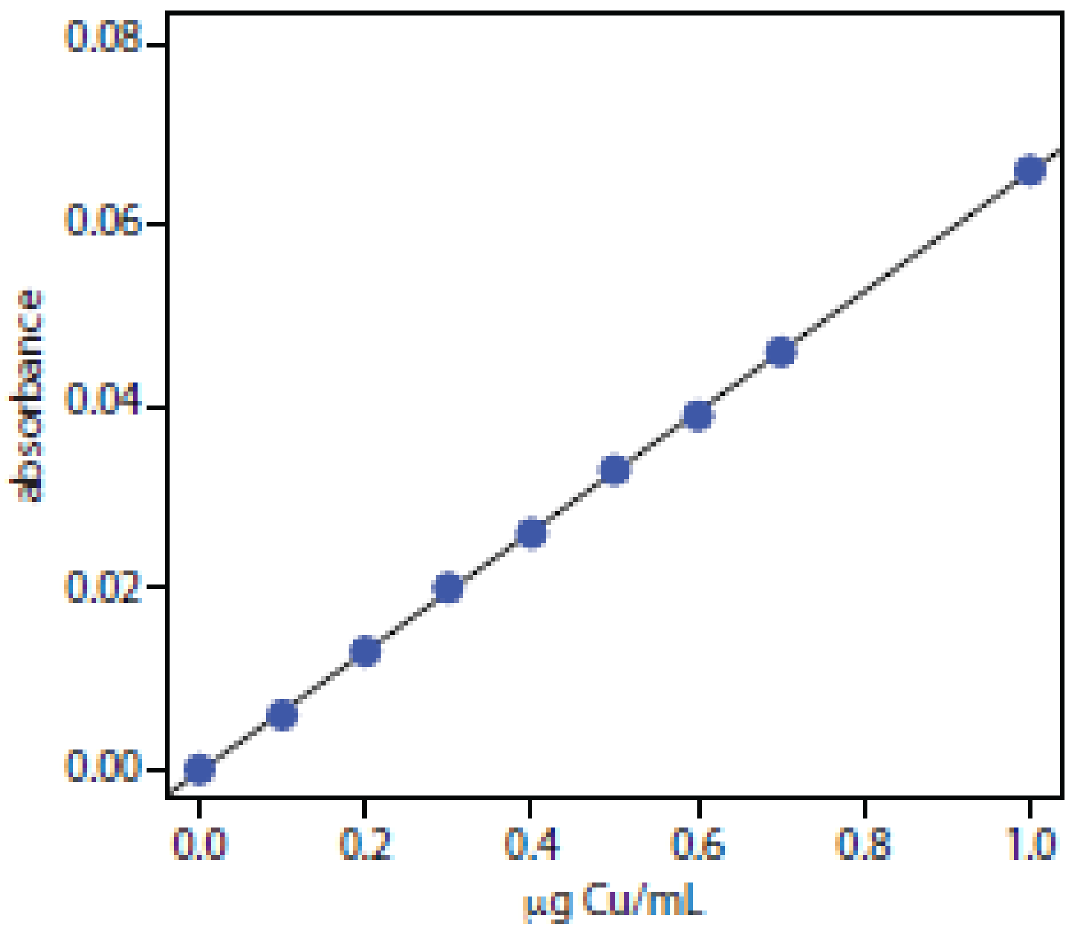


Linear regression

$$[Y] = [A][X]$$

$$\begin{bmatrix} 0.000 \\ 0.1 \\ 0.2 \\ 003 \\ 0.4 \\ 0.5 \\ 0.6 \\ 0.7 \\ 1.0 \end{bmatrix} = \begin{bmatrix} m & b \end{bmatrix} \begin{bmatrix} 0.000 \\ 0.006 \\ 0.013 \\ 0.020 \\ 0.023 \\ 0.033 \\ 0.039 \\ 0.046 \\ 0.066 \end{bmatrix}$$

Generalized Matrix Inverse

Given Linear map $A: \mathbb{R}^N \to \mathbb{R}^M$, $f \in \mathbb{R}^N$, $g \in \mathbb{R}^M$ and $A\vec{f} \in \mathbb{R}^M$

$$\boxed{\vec{g} = A\vec{f}}$$

data, model, state vector

Problem: Given A & $\vec{g}$, find $\vec{f}$ such that $A\vec{f}$ is "closest" to $\vec{g}$

Define: distance between $A\vec{f}$ & $\vec{g}$ is:

Misfit function, or *Residual*, or *Cost function*, or…

$$\epsilon = \|A\vec{f} - \vec{g}\|$$

It's a functional…

$$= \left[(A\vec{f} - \vec{g}) \cdot (A\vec{f} - \vec{g})\right]^{1/2}$$

Hint: Minimize ϵ^2… easier math!

Solution

- If $N = M$:

$A: \mathbb{R}^N \to \mathbb{R}^N$, then $\vec{f} = A^{-1}\vec{g}$, $\epsilon = 0$

(and $\det(A) \neq 0$)

- If $N < M$ (over constrained… more eqtns. than unknowns)

$$\Rightarrow \epsilon^2 = \|A\vec{f} - \vec{g}\|^2 = (A\vec{f} - \vec{g}) \cdot (A\vec{f} - \vec{g})$$

$$= A\vec{f} \cdot A\vec{f} - A\vec{f} \cdot \vec{g} - \vec{g} \cdot A\vec{f} + \vec{g} \cdot \vec{g}$$

Notes:

(1) $A\vec{f} \cdot \vec{g} = \vec{g} \cdot A\vec{f}$ (2) $A\vec{f} \cdot A\vec{f} = A^T A \vec{f} \cdot \vec{f}$ (3) $A^T A = (A^T A)^T$

so

$$\epsilon^2 = \underbrace{A^T A\,\vec{f}\cdot\vec{f}}_{\text{Like } A\vec{x}\cdot\vec{x}} - \underbrace{2A\vec{f}\cdot\vec{g}}_{\text{Like } A\vec{x}\cdot c} + \underbrace{\|g\|^2}_{\text{Like } c}$$

use the derivative table!

$$\frac{\partial \epsilon^2}{\partial f_k} = \vec{e}_k\cdot\Big(\underbrace{A^T A + (A^T A)^T}_{2A^T A}\Big)\vec{f} - 2\vec{e}_k\cdot\left(A^T\vec{g}\right) + 0$$

$$= \vec{e}_k\cdot\left(2A^T A\vec{f} - 2A^T\vec{g}\right)$$

which we set equal to zero to minimize! (for all k)

$$\Rightarrow 2A^T A\vec{f} - 2A^T\vec{g} = 0$$

$$\Rightarrow \underbrace{A^T A}_{\substack{\text{square!}\\ \text{(and symmetric)}}}\,\vec{f} = A^T\underbrace{\vec{g}}_{\text{given}}$$

find $\vec{f}$...

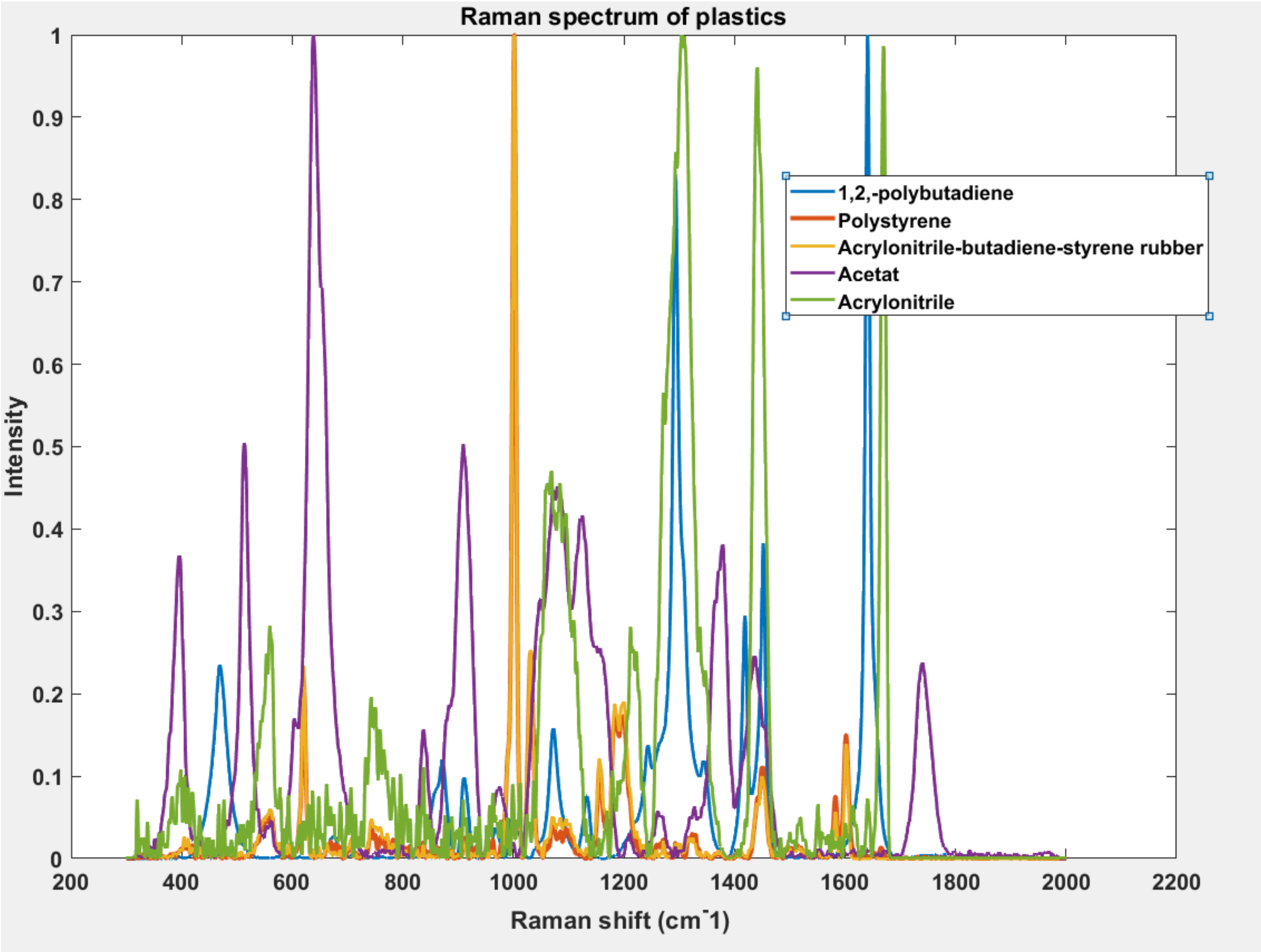
$$\boxed{\vec{f} = (A^T A)^{-1} A^T\vec{g}}$$

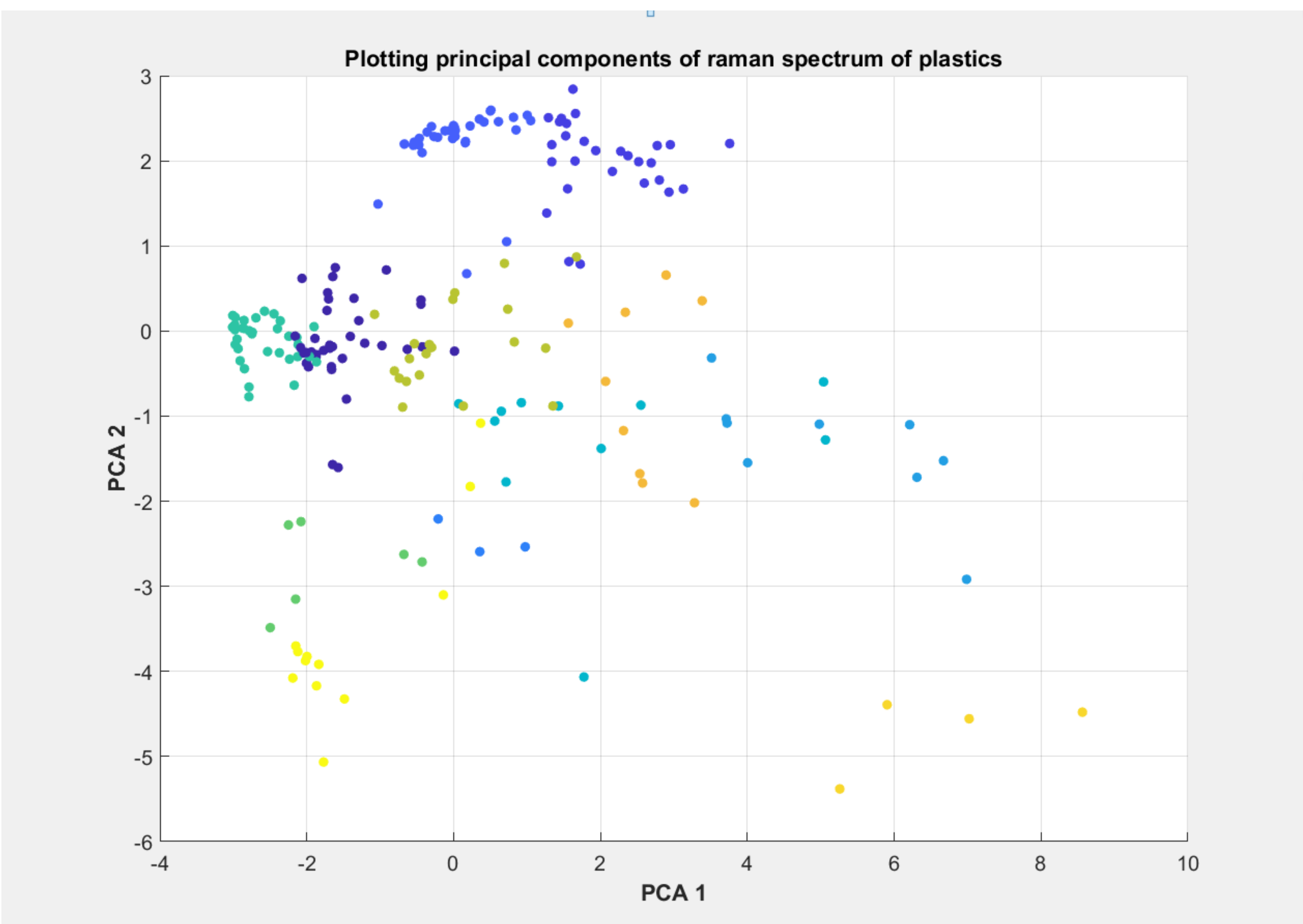
Generalized Matrix Inverse

(for overconstrained stuff)

Sometimes its easier to do it in other basis sets

- You can transform data from one space to another
- Think of it like fourier transforms in a way
- Singular value decomposition or principal component analysis
- For large multivariate models take the data and condense it down to a space where the first n variables contain the majority of the variation


Raman spectrum of plastics
Intensity
Raman shift (cm¯1)
1,2,-polybutadiene
Polystyrene
Acrylonitrile-butadiene-styrene rubber
Acetat
Acrylonitrile


Plotting principal components of raman spectrum of plastics
PCA 2
PCA 1