Active analysis of chemical mixtures with multi-modal non-negative least squares

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perception sensing instrumentation lab

Overview

Introduction

- What is active sensing?
- Infrared Fabry-Perot interferometry

Methods

- Non-negative least squares
- Multi-modal search
- Wavelength selection

Results

- Chemical dataset
- System behavior
- Comparison with passive sensing

Discussion

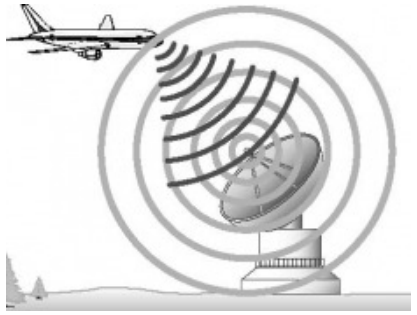
What is active sensing?

Perception is an active process

– "We not only see but we look, we not only touch we feel"

-J.J. Gibson

Active sensor vs. active sensing



– **Active sensor**: a device that transmits energy in order to make measurements

  - E.g., radar, sonar

– **Active sensing**: a control strategy that dynamically adapts the sensor's configuration as it interacts with the environments

  - E.g., changing camera viewpoints

What is active sensing?

Analogy

- Guessing games
  - 20 questions, Pictionary, Battleship, Yes and no, Hangman

Question	Answer
Is your character real?	Yes
Is your character male?	Yes
Is he alive?	Yes
Is he an actor?	No
Is he linked with sports?	No
Is he a musician?	Yes
Is he more than 50 years old?	Yes
Does he play the guitar?	Yes
Is he American?	Yes
Does he wear headgear?	Yes
Does he have messy hair?	Yes
Is it Bob Dylan?	Yes

Vague

Specific

What is active sensing?

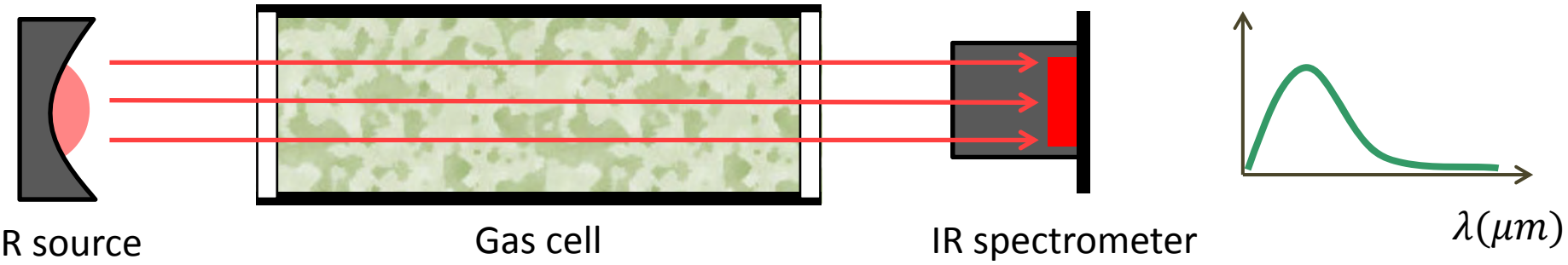
Analogy

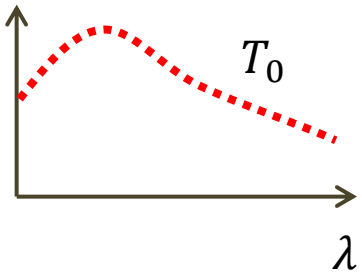
- Guessing games
  - 20 questions, Pictionary, Battleship, Yes and no, Hangman
- Two seemingly conflicting problems at the same time
  - Find the right answer
  - Ask the right questions
- Advantage
  - Incorporate decision early in the signal processing pipeline
  - Reduce sensing costs ($, energy, time, computing power)
  - Lower sensor requirements

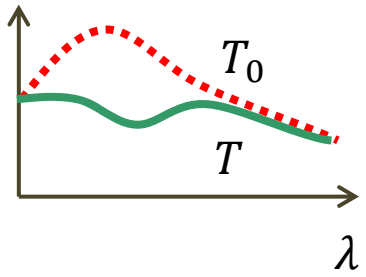
Prior work

Chemical	Identity	Concentration	Sensor	Reference
Single	Unknown	Fixed	MOX	Gosangi et al. 2010 *IEEE Sensors J*
Single	Unknown	Unknown (continuous)	FPI	Huang et al. 2012 *IEEE Sensors J*
Mixture	Known	Unknown (discrete)	MOX	Gosangi et al. 2013 *S&A B: Chemical*
Mixture	**Unknown**	**Unknown (continuous)**	**FPI**	**Huang et al. 2013 *ICASSP***

Infrared absorption spectroscopy

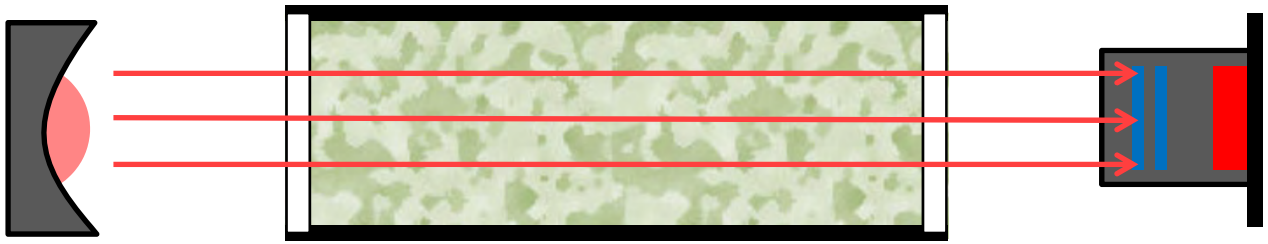


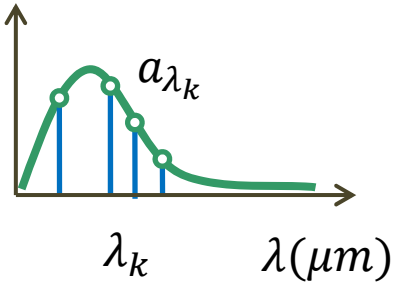




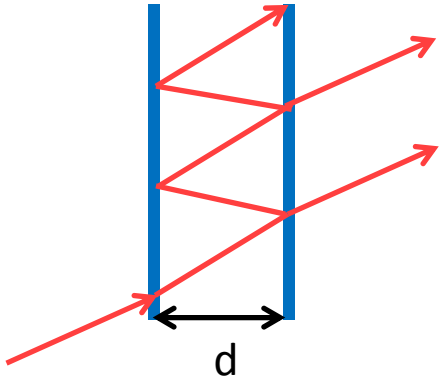
$$A = -\log_{10}\frac{T}{T_0}$$

Fabry-Perot interferometer





$$A_i = [a_{i\lambda_1}, \ldots, a_{i\lambda_n}]^T$$



$$\lambda = f(d)$$

IR absorption

Properties

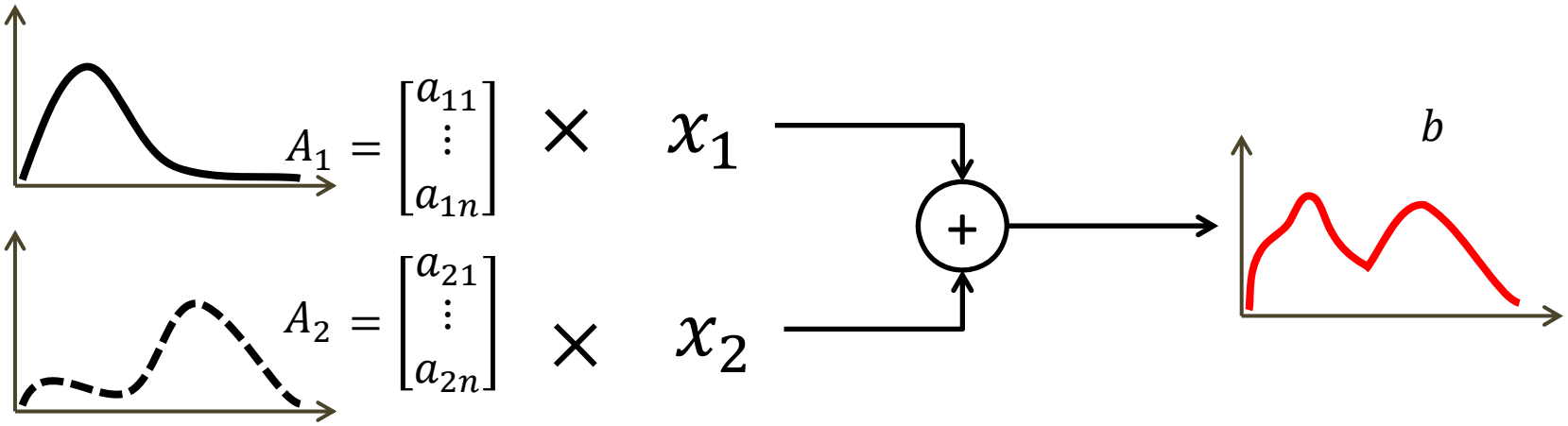
– Absorption spectrum is linear (Beer's law)

$$\sum_{i=1}^{p} A_i x_i = b$$

Absorption spectrum of each chemical A_i

Concentration of each chemical x_i

Absorption spectrum b of the mixture

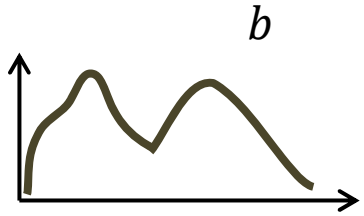


Traditional mixture analysis

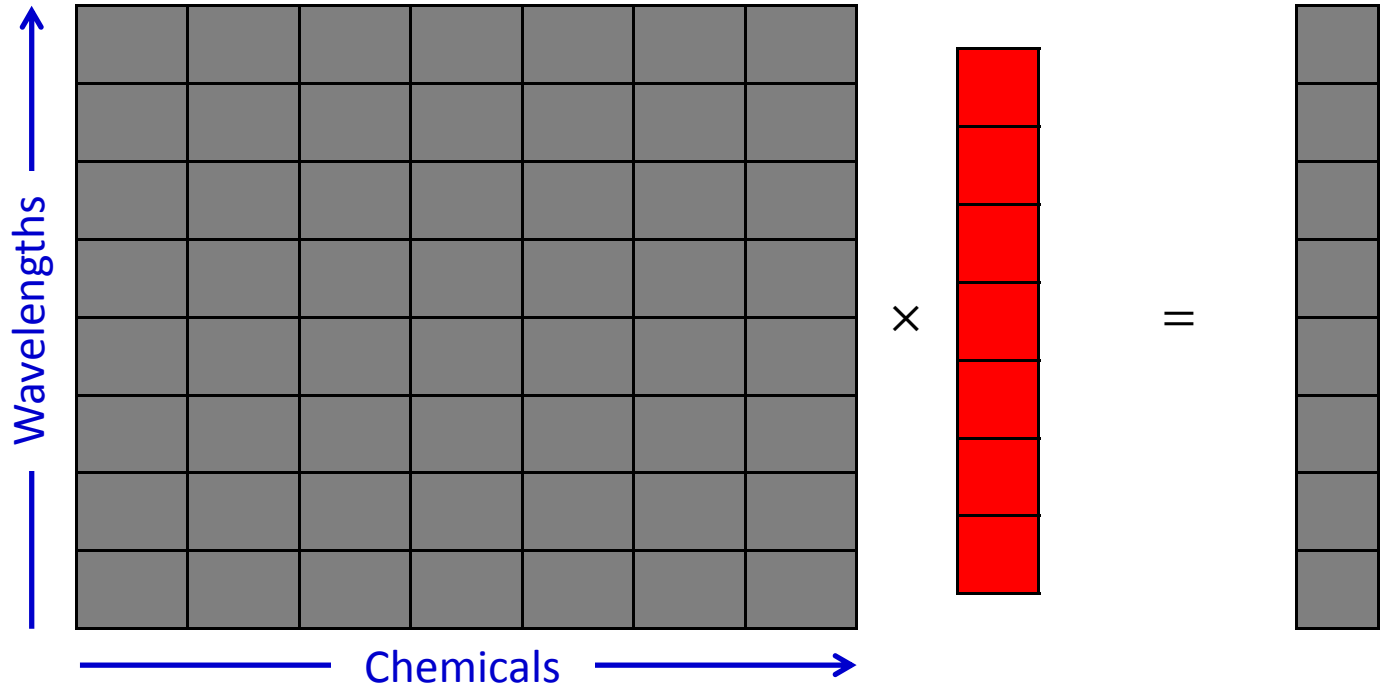
Problem definition

– Estimate x, **given b (all wavelengths)**

$$Ax = b$$
$$s.t.: x \geq 0$$



$A\ (n \times p)$ $x\ (p \times 1)$ $b\ (n \times 1)$

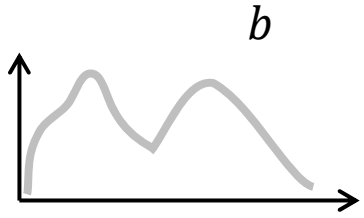


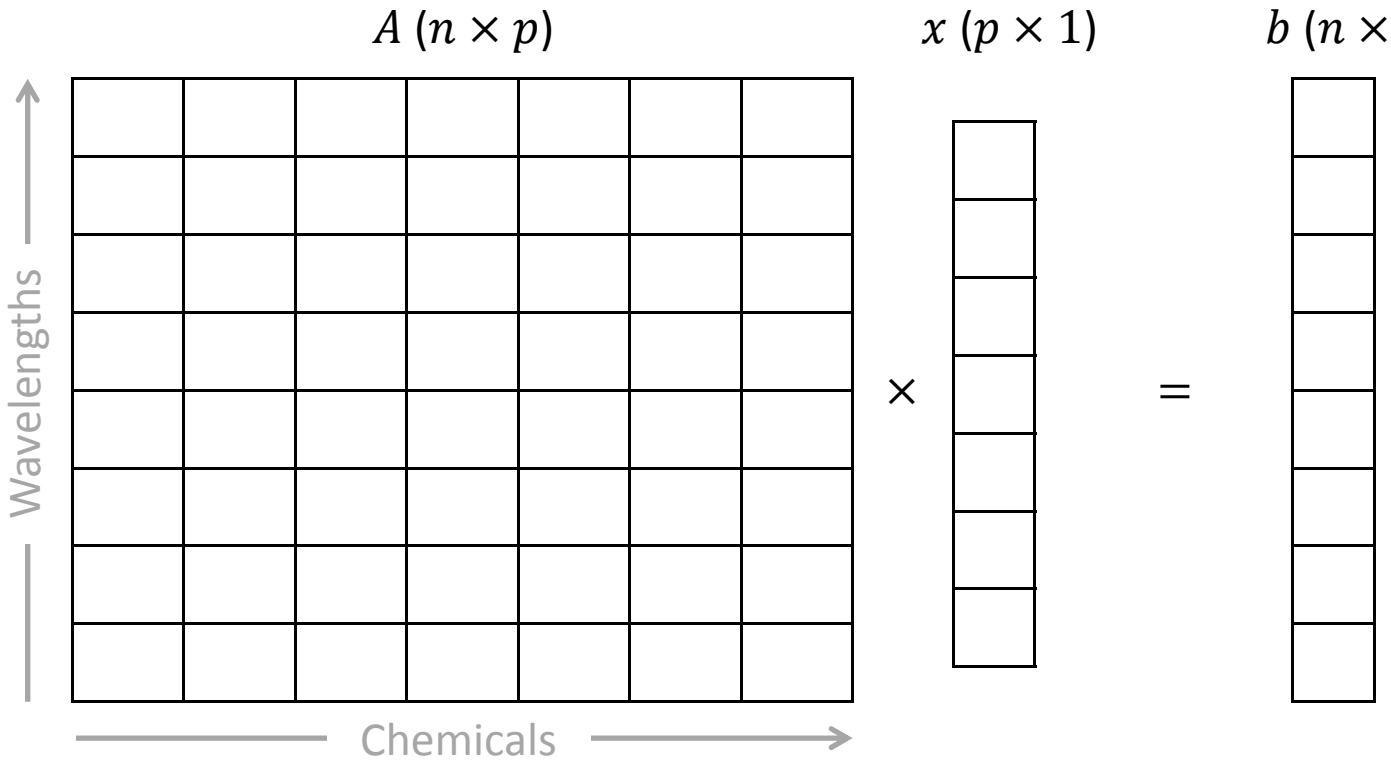
Active mixture analysis

Problem definition

– Estimate x, **but measuring one wavelength at a time**

$$Ax = b$$
$$s.t.: x \geq 0$$



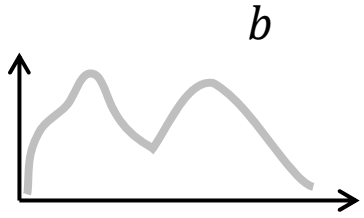


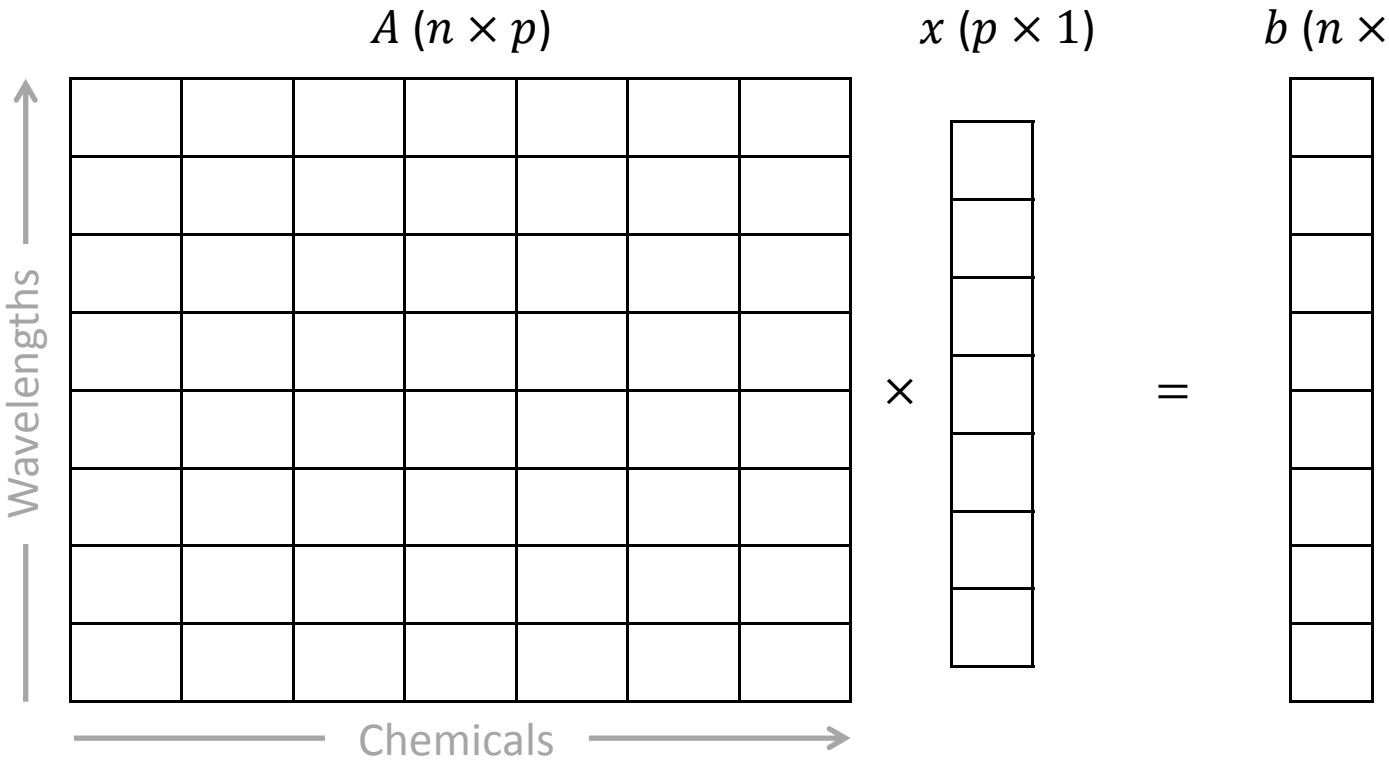
Active mixture analysis

Problem definition

– Select the best wavelengths in b to solve $Ax = b$

$$Ax = b$$
$$s.t.: x \geq 0$$



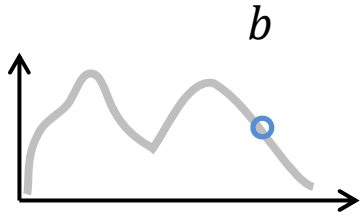


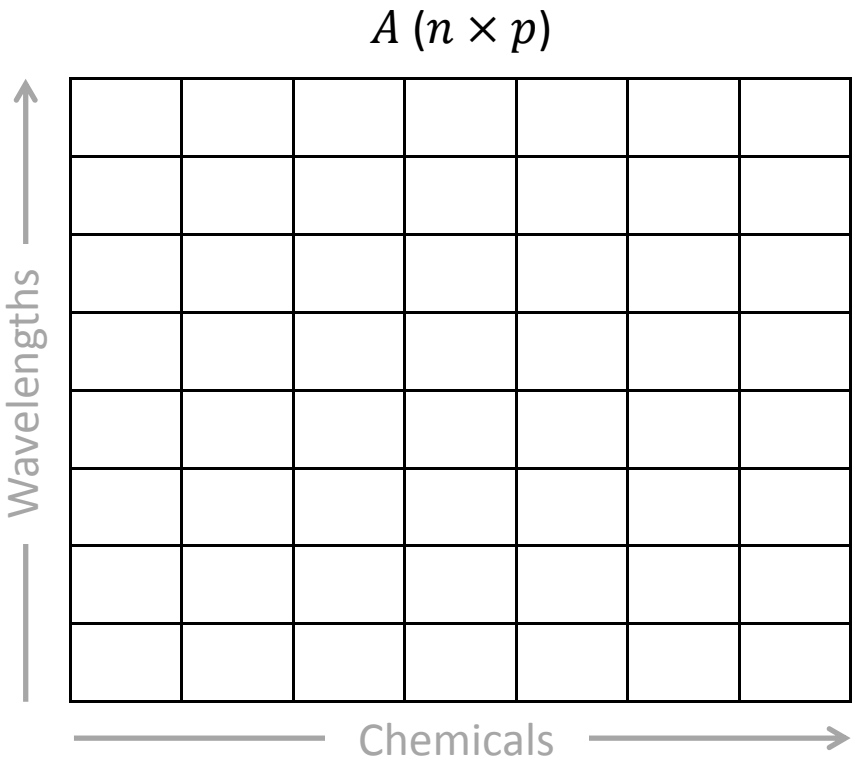
Active mixture analysis

Interpretation

– Each wavelength equals one element in b

$$Ax = b$$
$$s.t.: x \geq 0$$

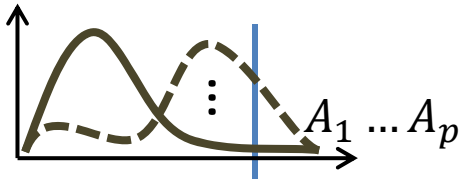




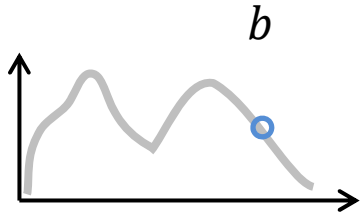
Active mixture analysis

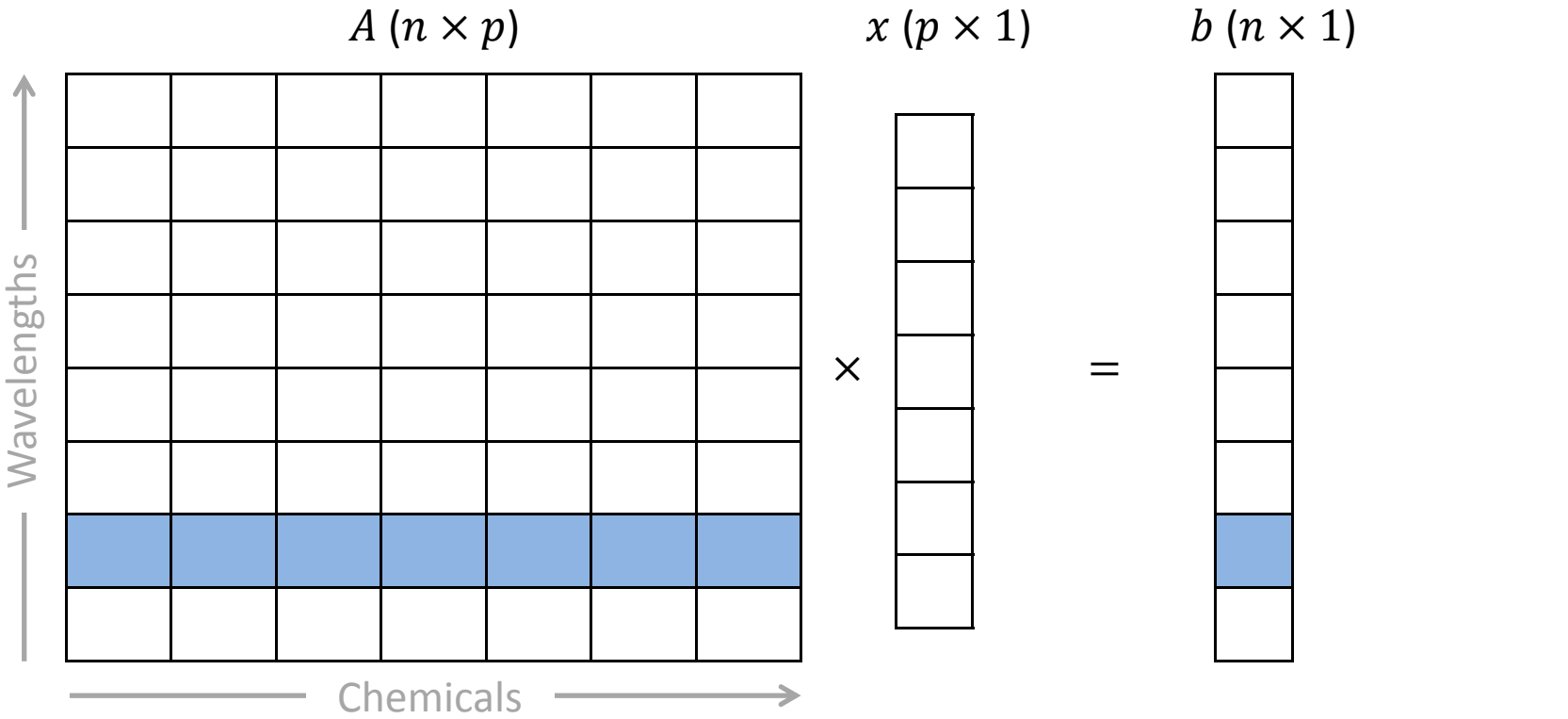
Interpretation

– Which allows us to use an additional row in A



$$Ax = b$$
$$s.t.: x \geq 0$$

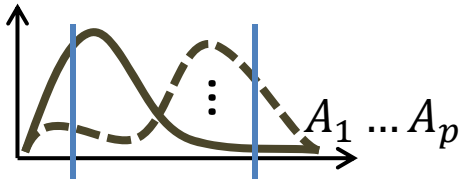




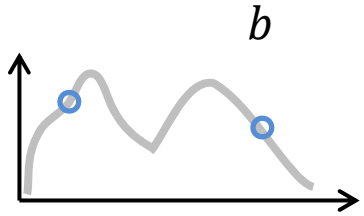
Active mixture analysis

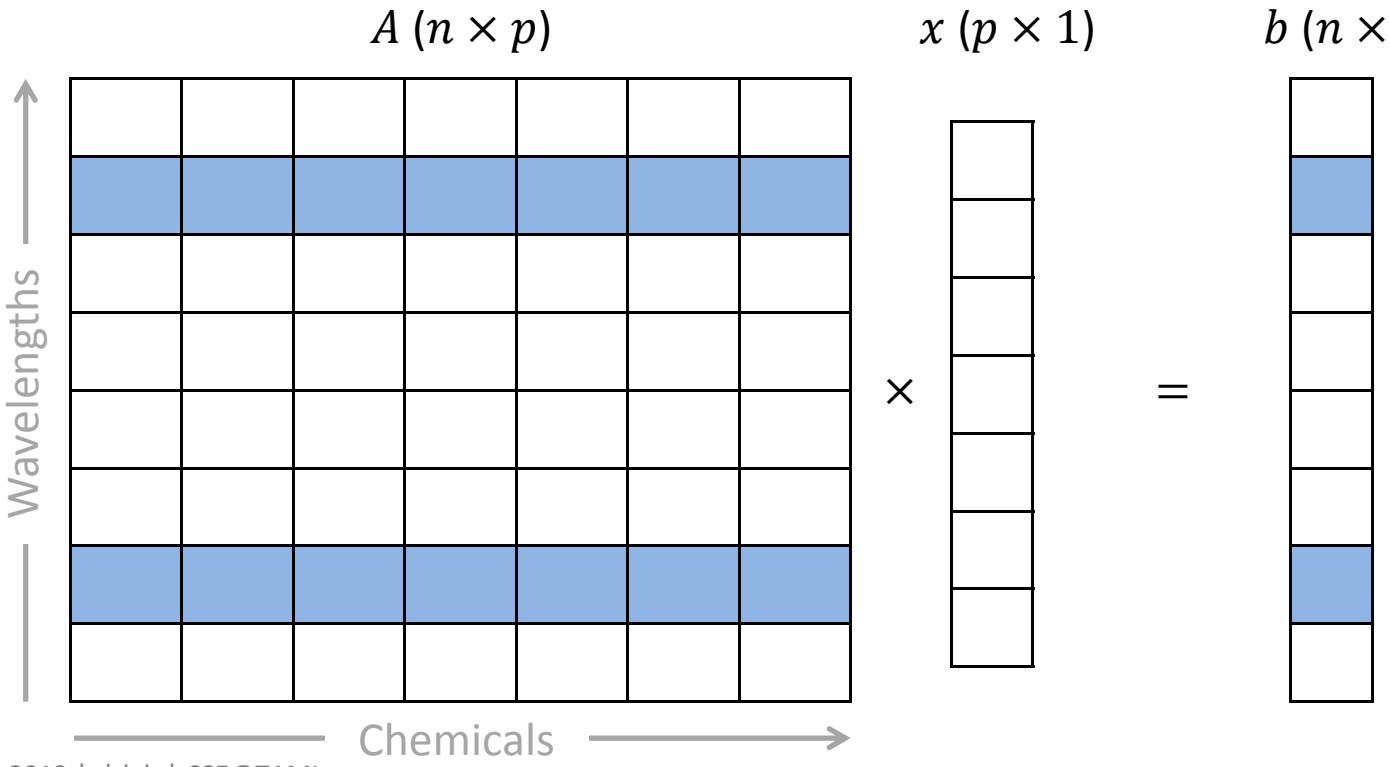
Interpretation

– Each new wavelength adds a new row in A



$$Ax = b$$
$$s.t.: x \geq 0$$

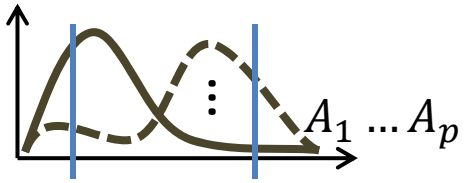




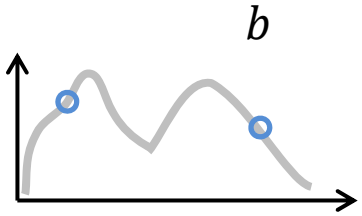
Active mixture analysis

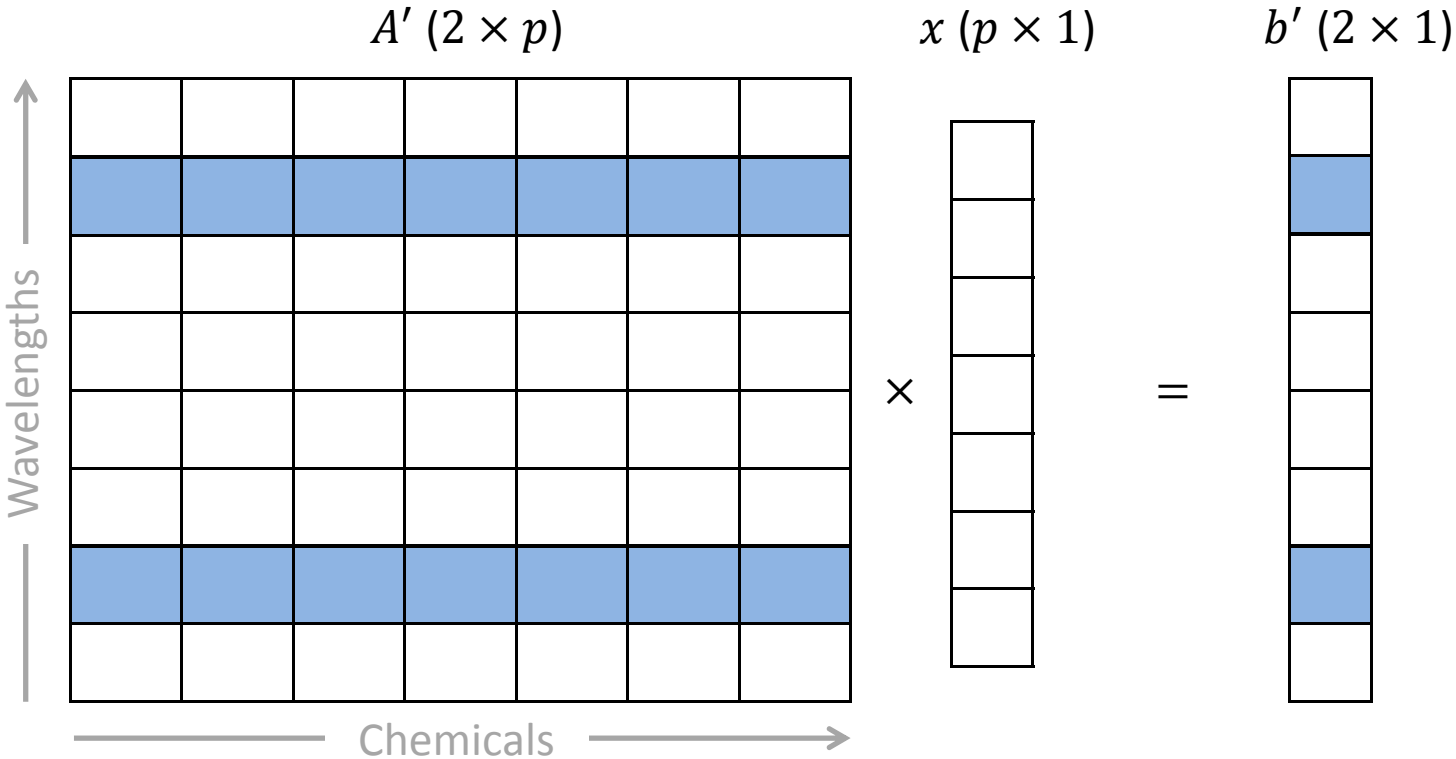
Issue

– The underlying linear system may be under-determined



$$A'x = b'$$
$$s.t.: x \geq 0$$



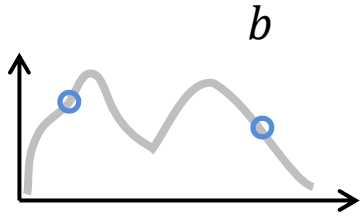


Active mixture analysis

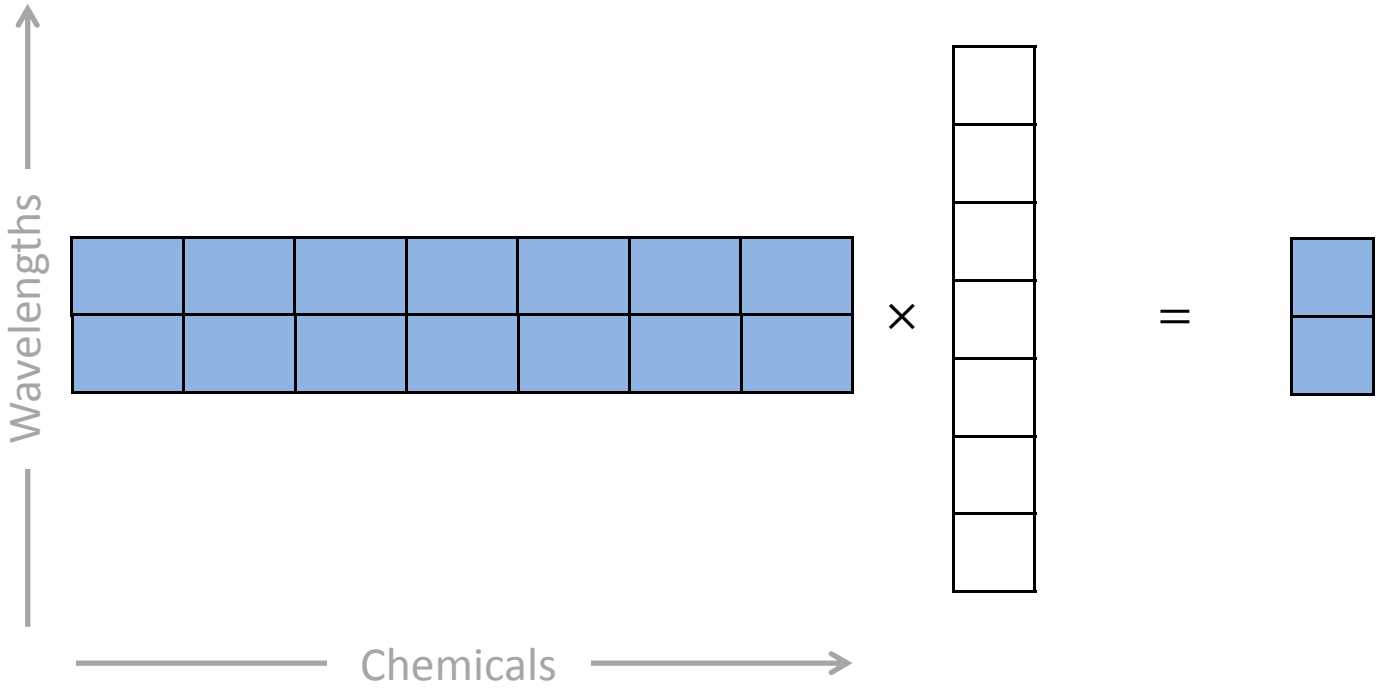
Solution

– Assume that x is sparse

$$A'x = b'$$
$$s.t.: x \geq 0$$



$A'\ (2 \times p)$ $\quad x\ (p \times 1)$ $\quad b'\ (2 \times 1)$

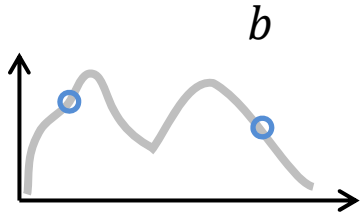


Active mixture analysis

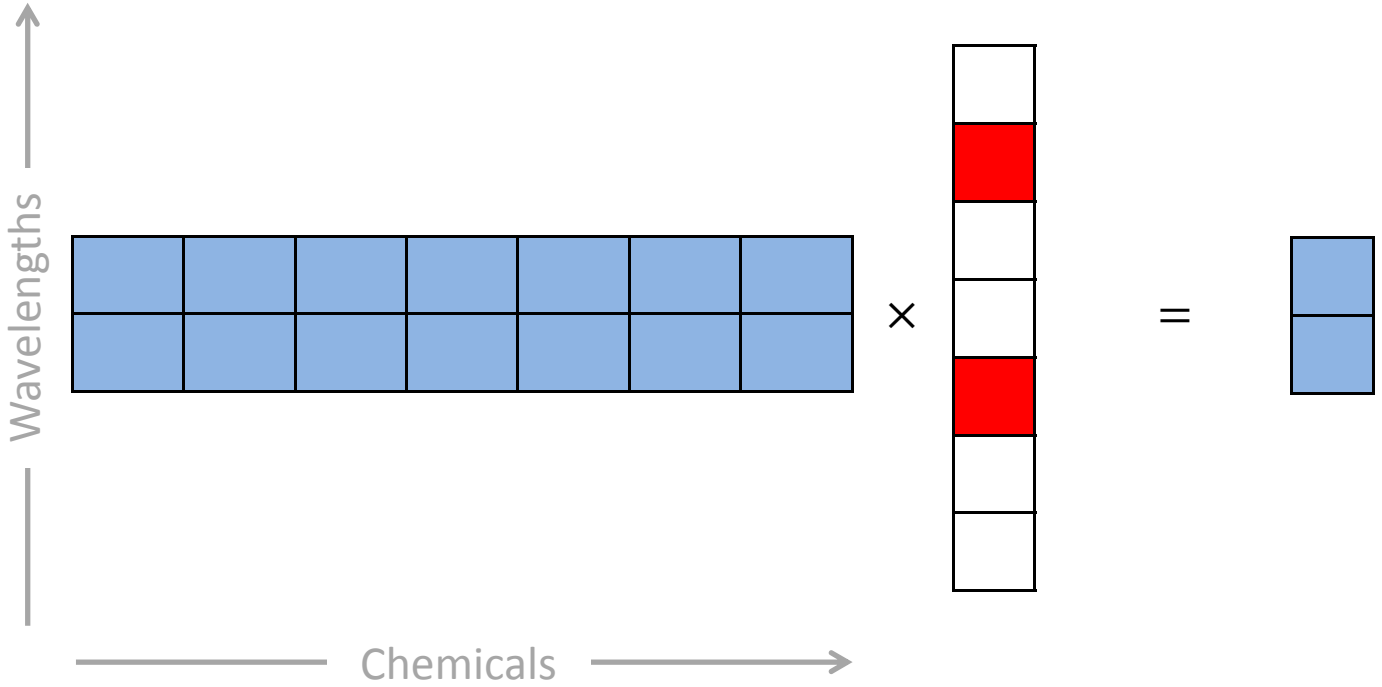
Subset selection

– Select 1-2 elements in x

$$A'x = b'$$
$$s.t.: x \geq 0$$



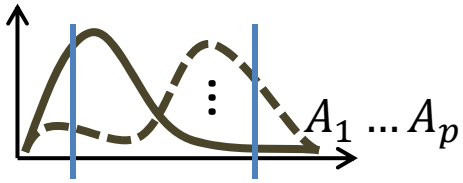
$A'\ (2 \times p)$ $\quad$ $x\ (p \times 1)$ $\quad$ $b'\ (2 \times 1)$



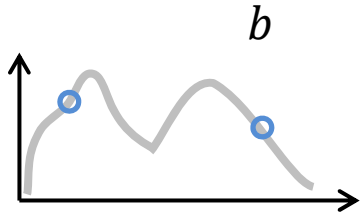
Active mixture analysis

Interpretation

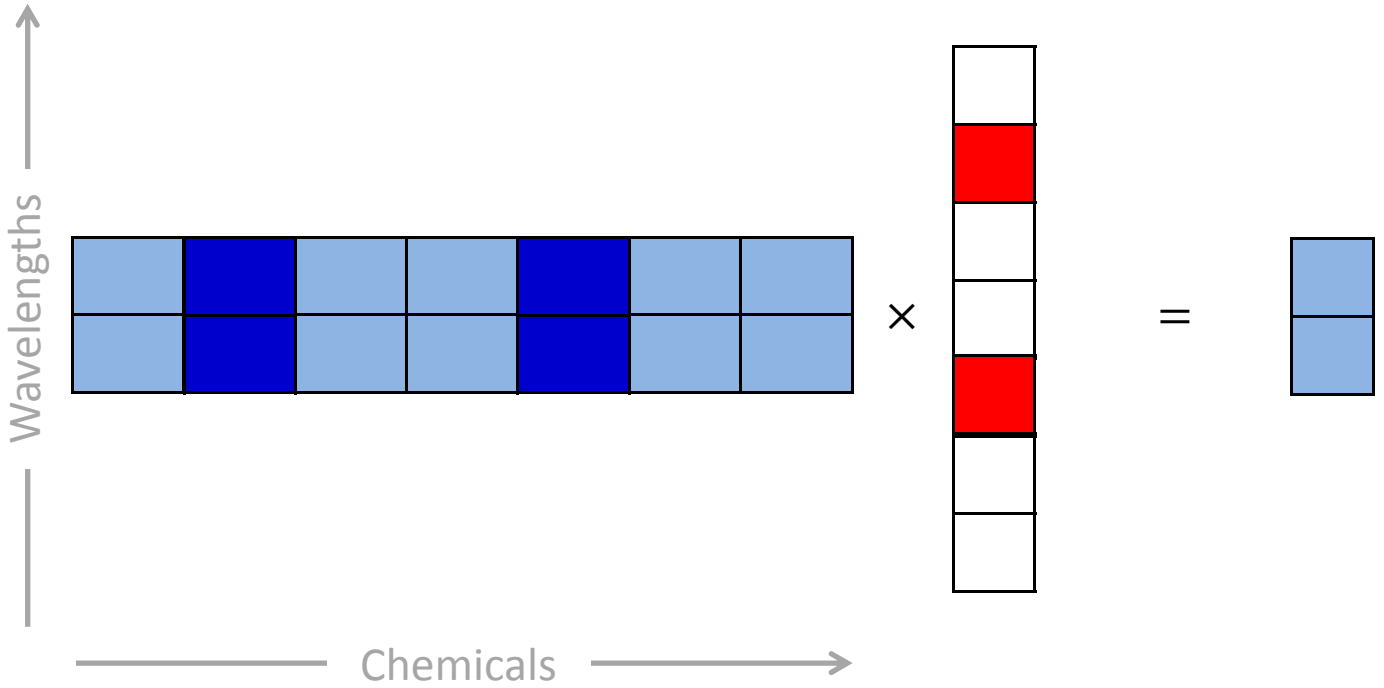
– One element in x implies one column in A



$$A'x = b'$$
$$s.t.: x \geq 0$$



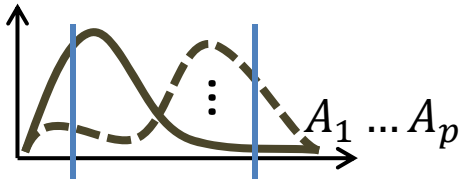
$A'\ (2 \times p)$ $\quad x\ (p \times 1)$ $\quad b'\ (2 \times 1)$



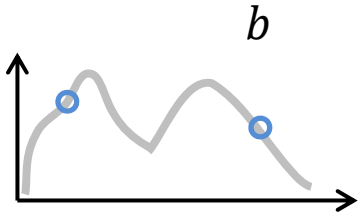
Active mixture analysis

The selection is not unique

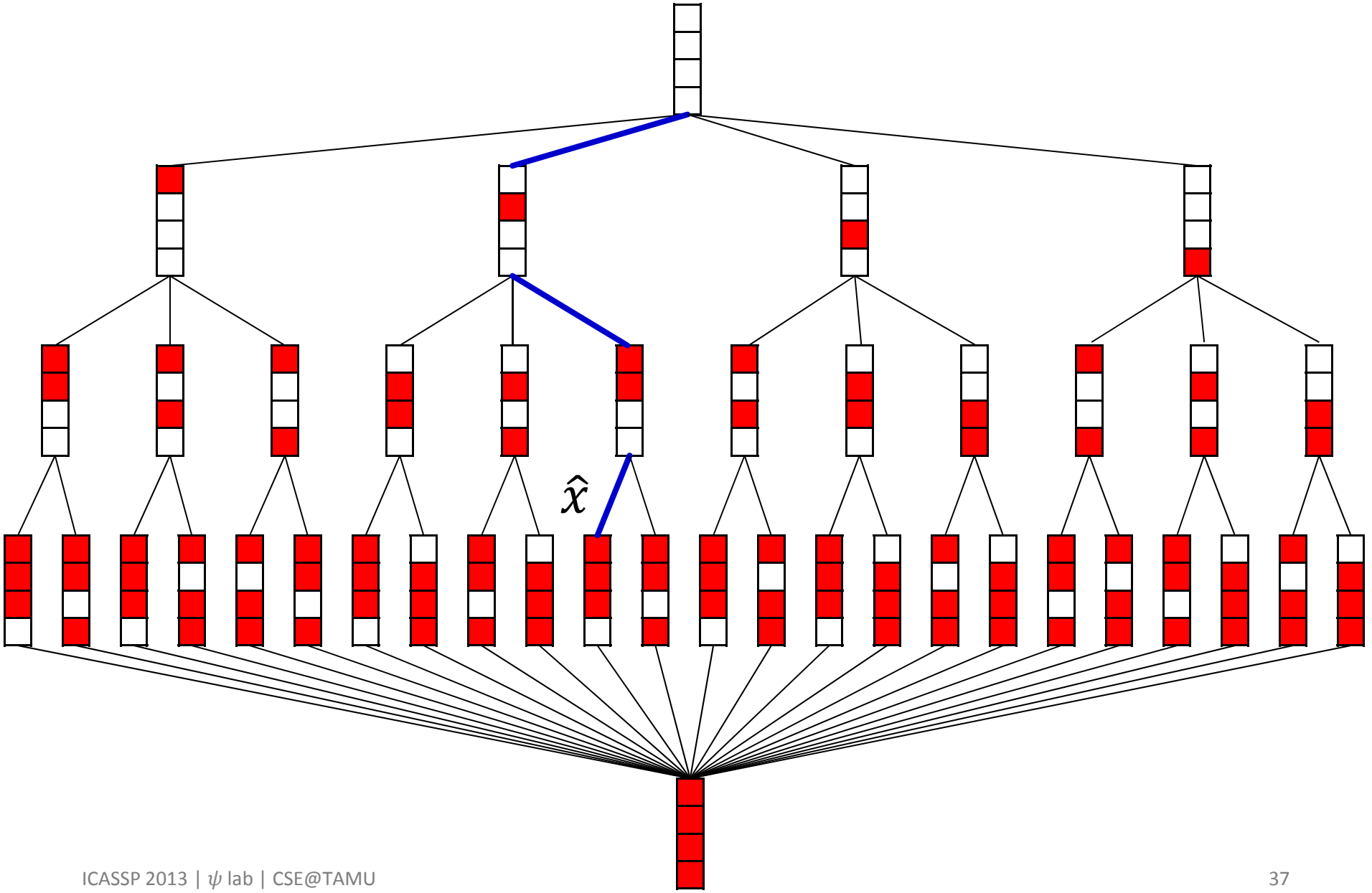
– A combinatorial problem ⇒ **search**



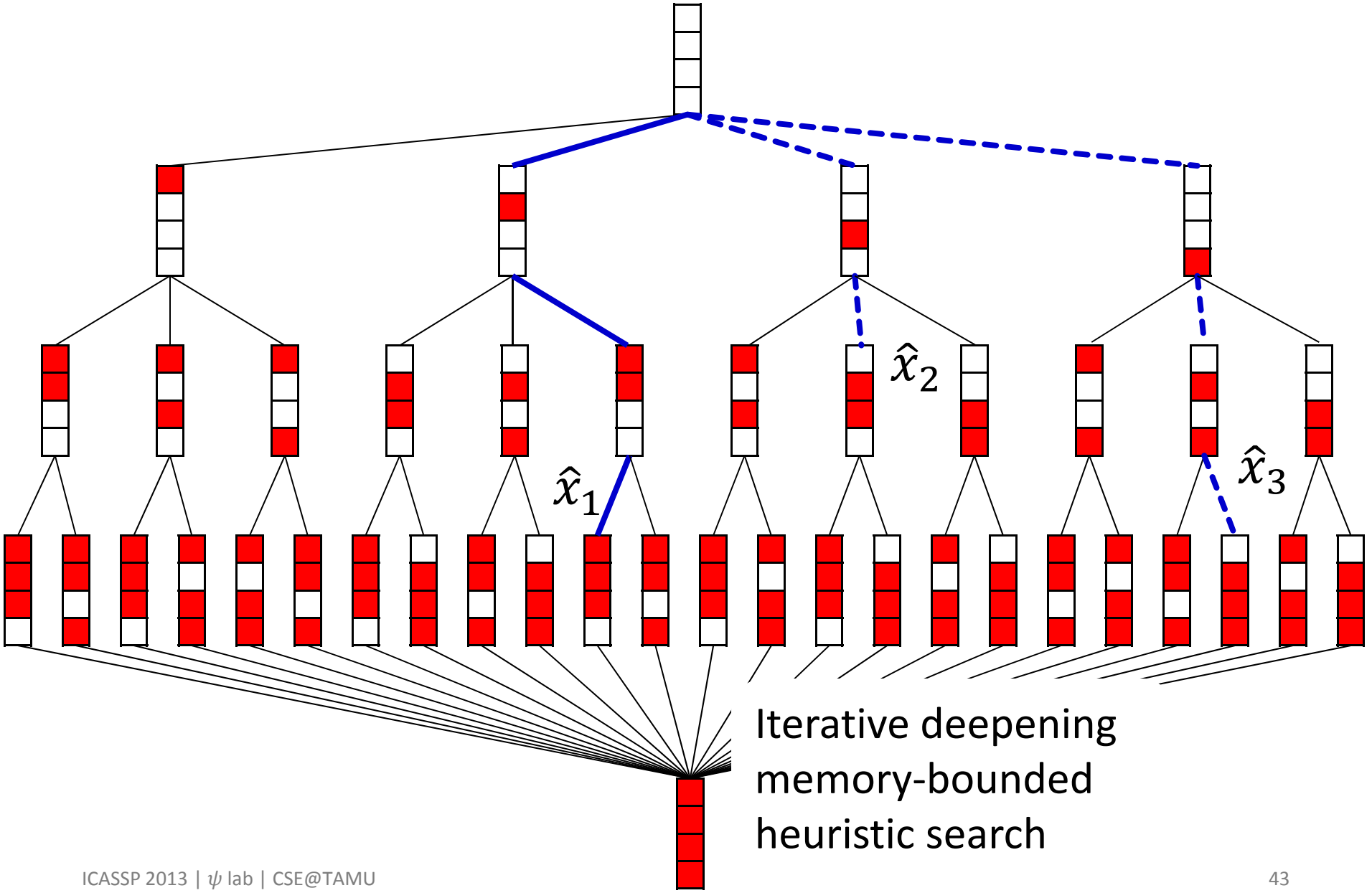
$$A'x = b'$$
$$s.t.: x \geq 0$$



Unimodal candidate selection

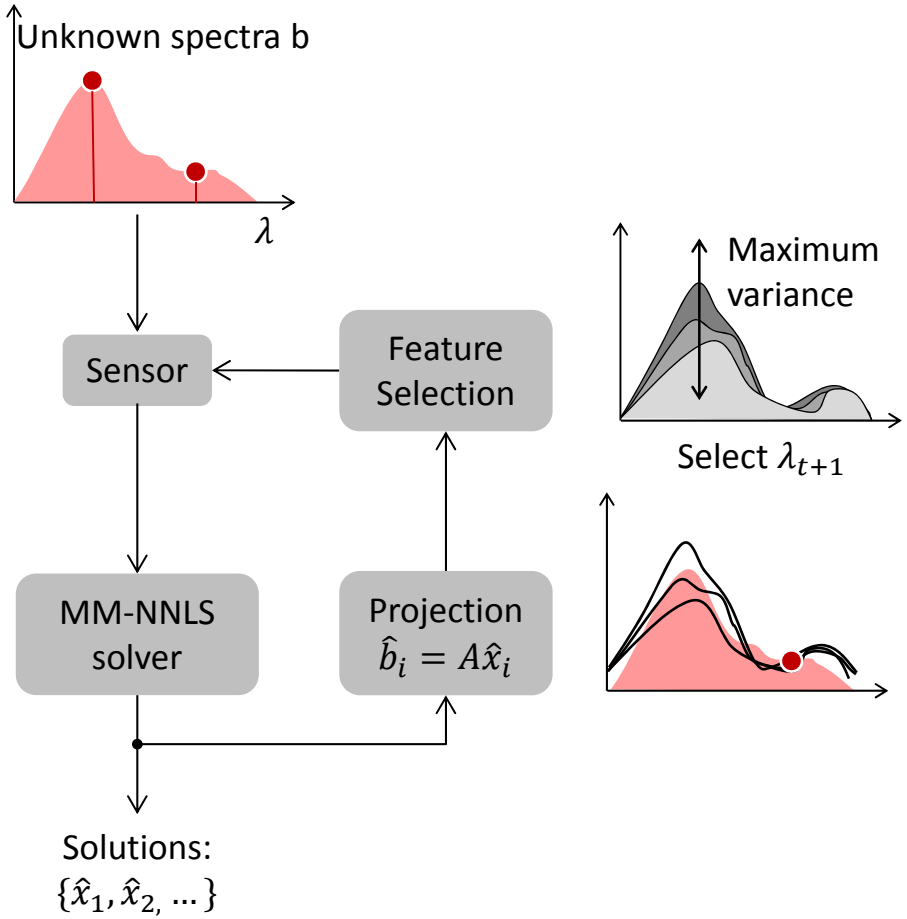


Multimodal candidate selection



Iterative deepening memory-bounded heuristic search

Wavelength selection



Case study

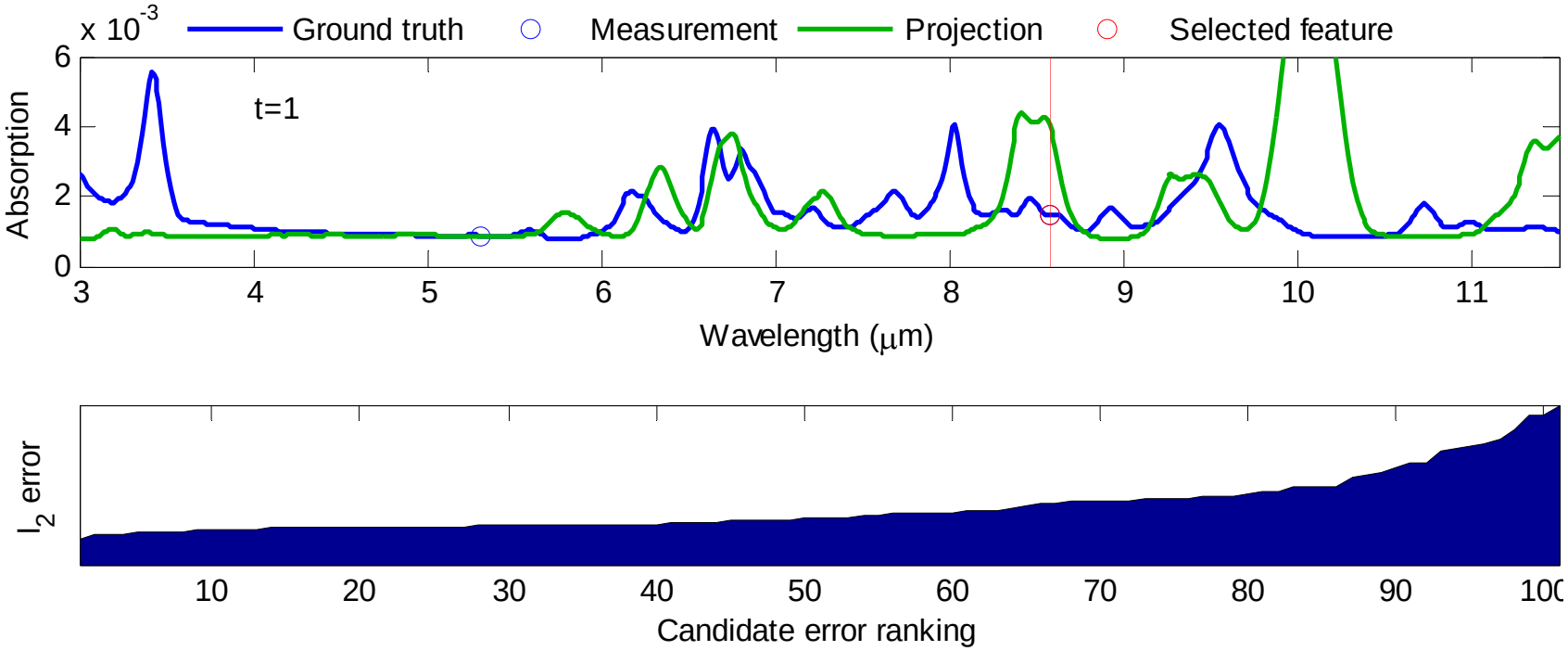
Dataset

- 100 chemicals from NIST WebBook (randomly chosen)
- Wavelength range: $3 - 11.5\mu m$
- Downsampled to 660 spectral lines
- Added 2% Gaussian noise

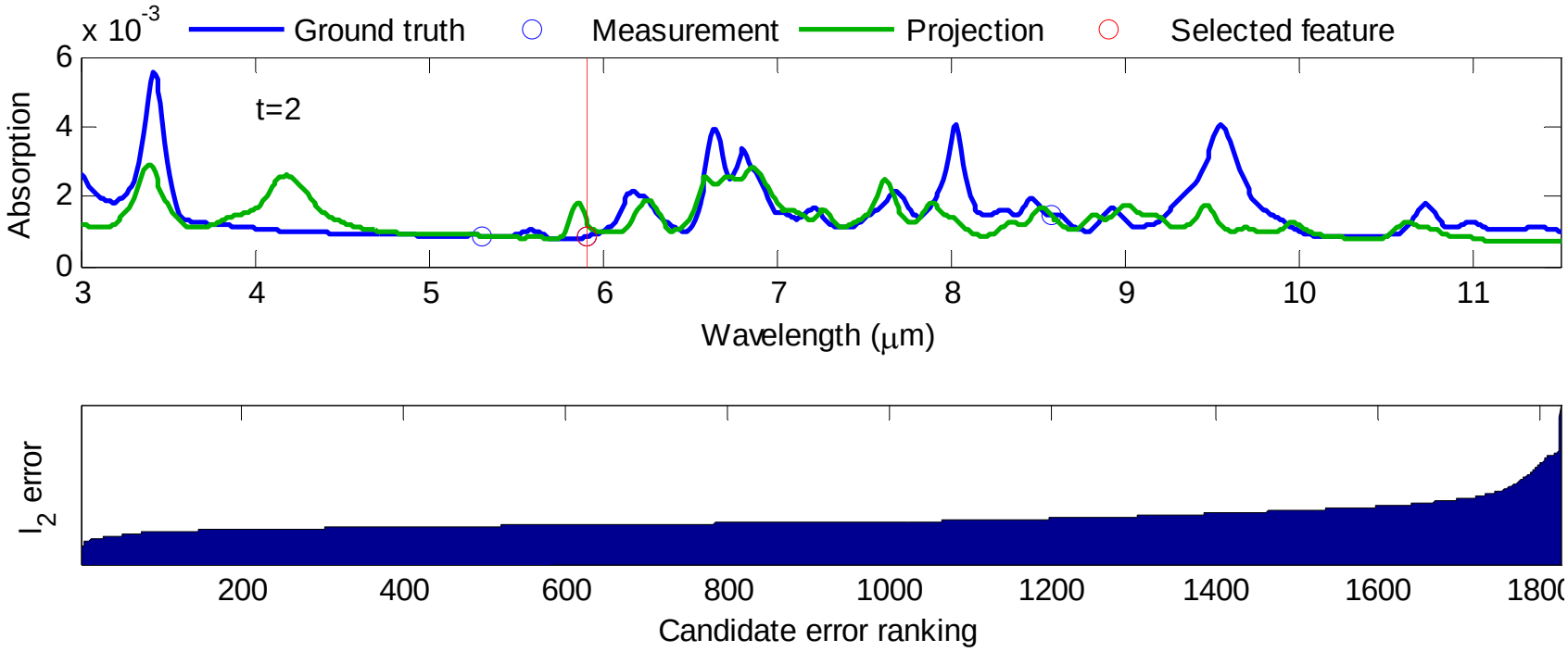
Setup

- 3 chemicals mixture (sparsity 3%)
- Search space $100^3 = 10^6$
- We consider up to 10^4 alternate paths

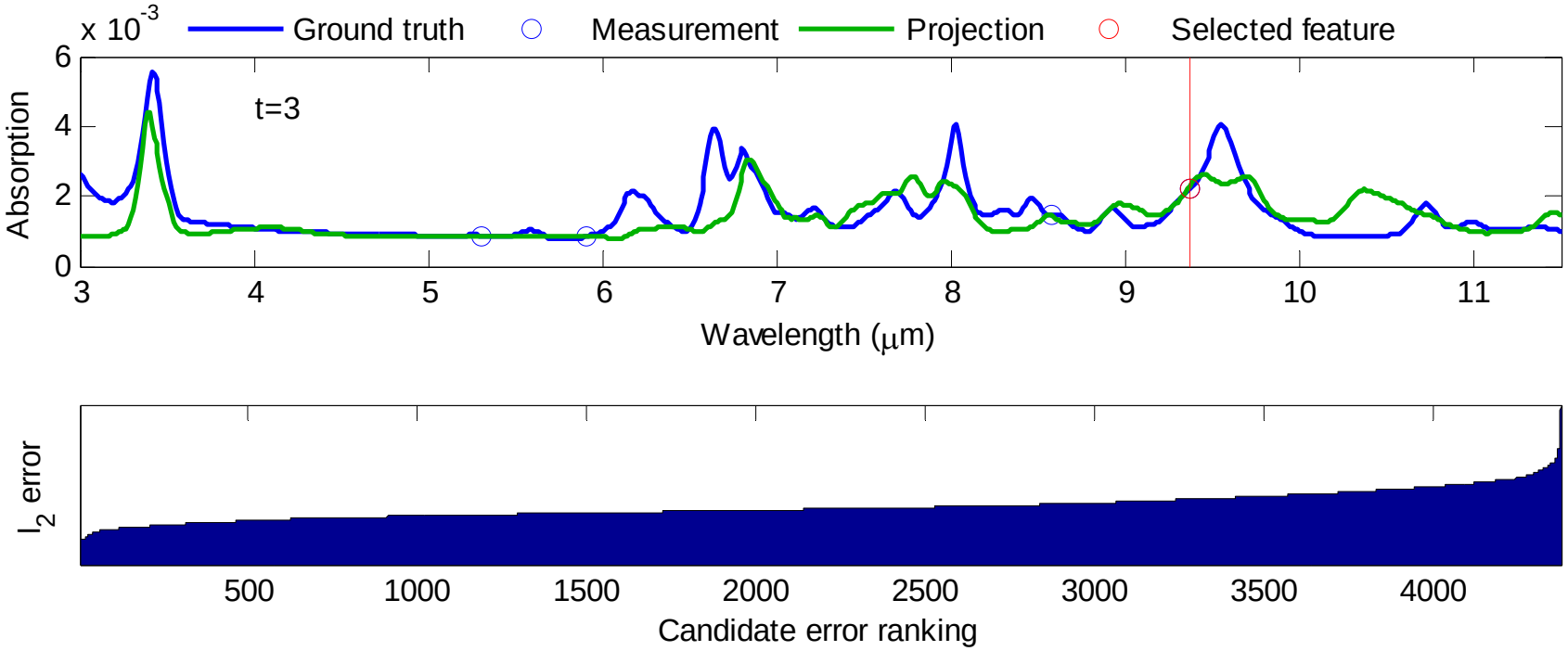
Step 1


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=1
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

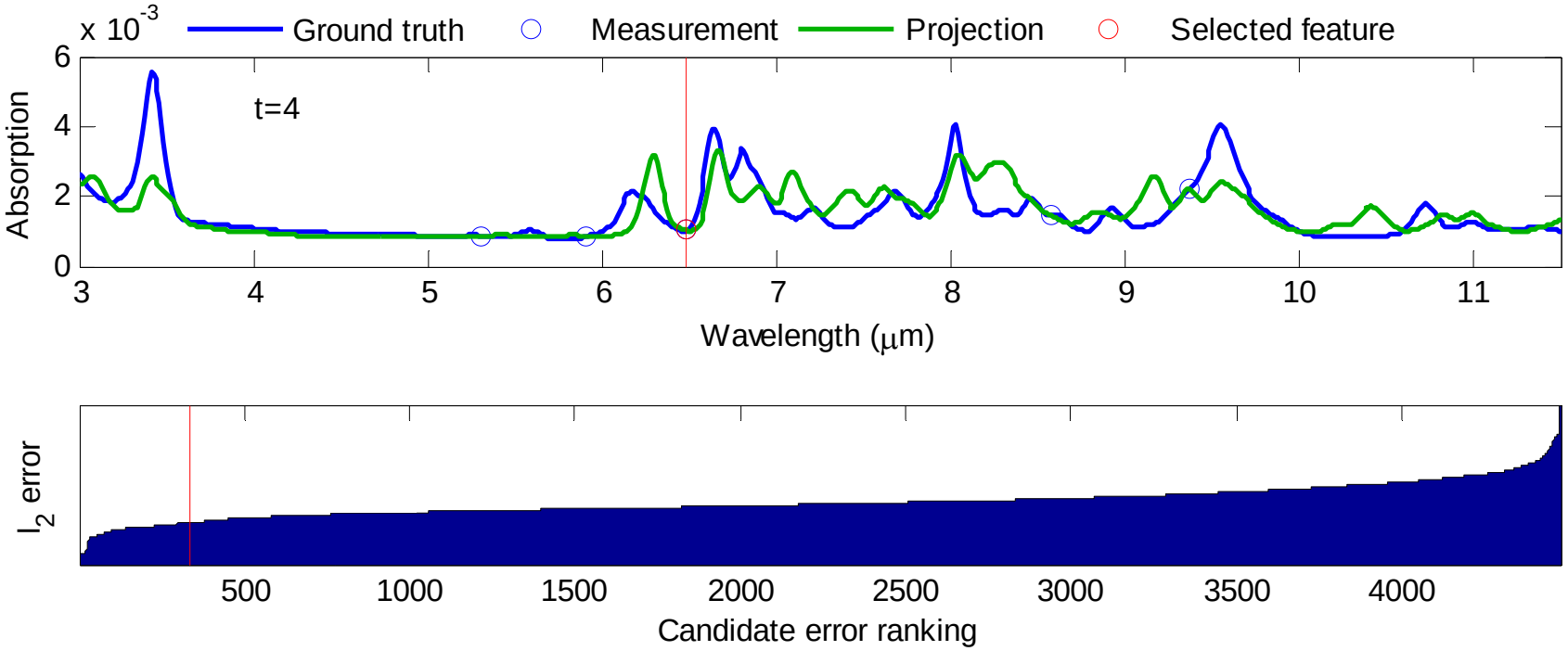
Step 2


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=2
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

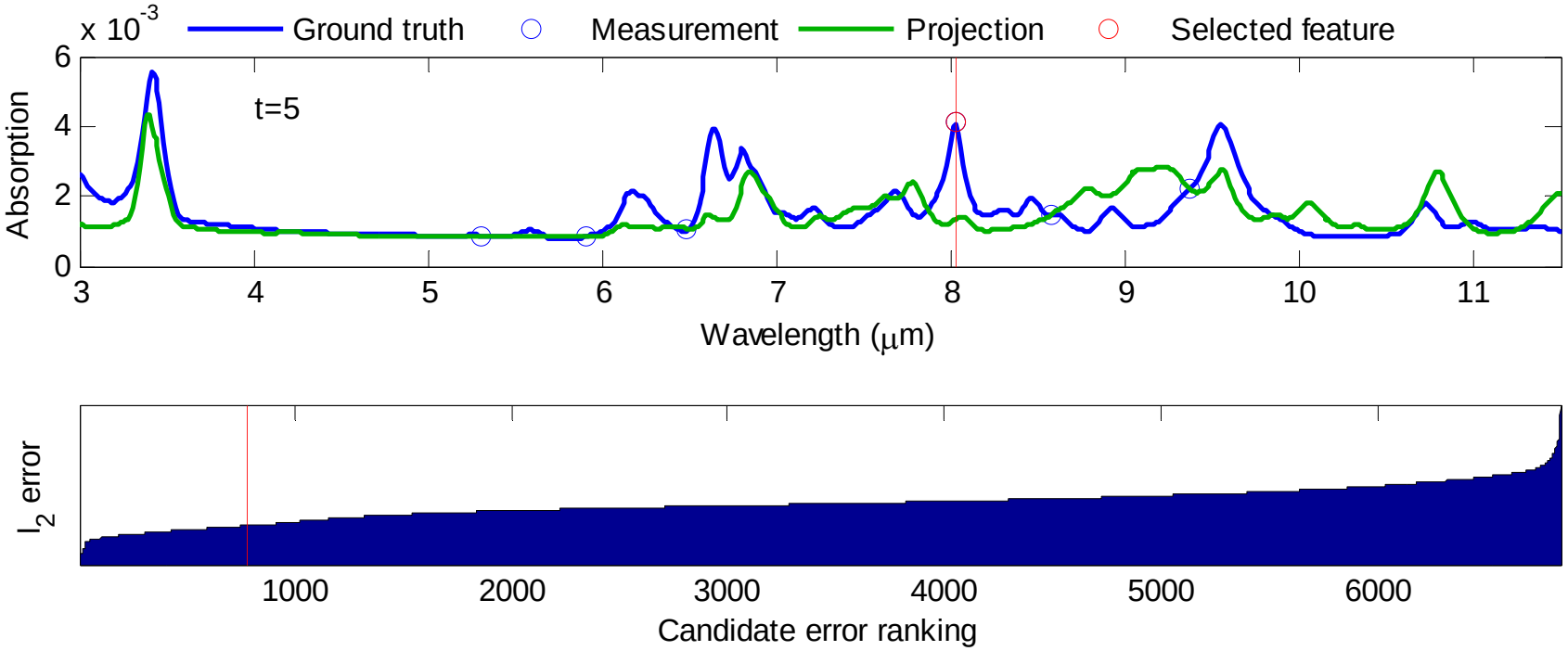
Step 3


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=3
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

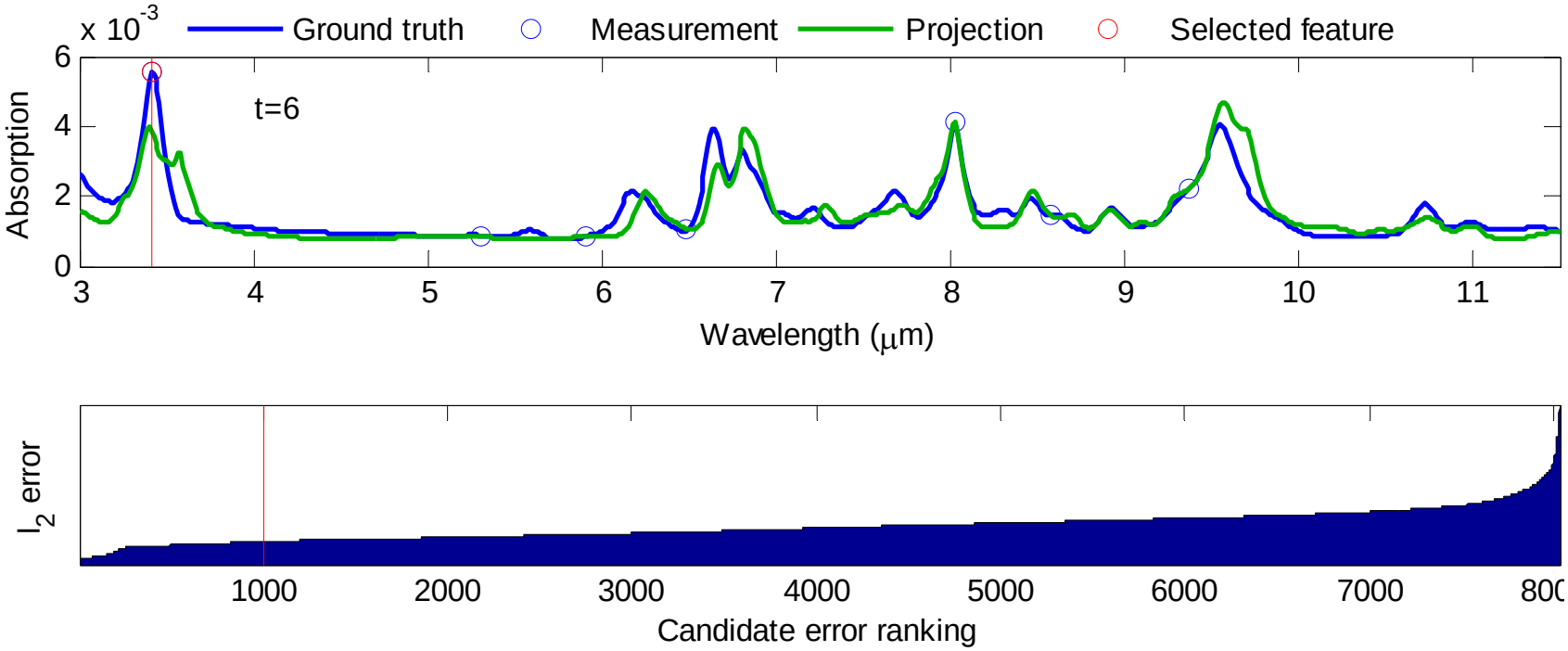
Step 4


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=4
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

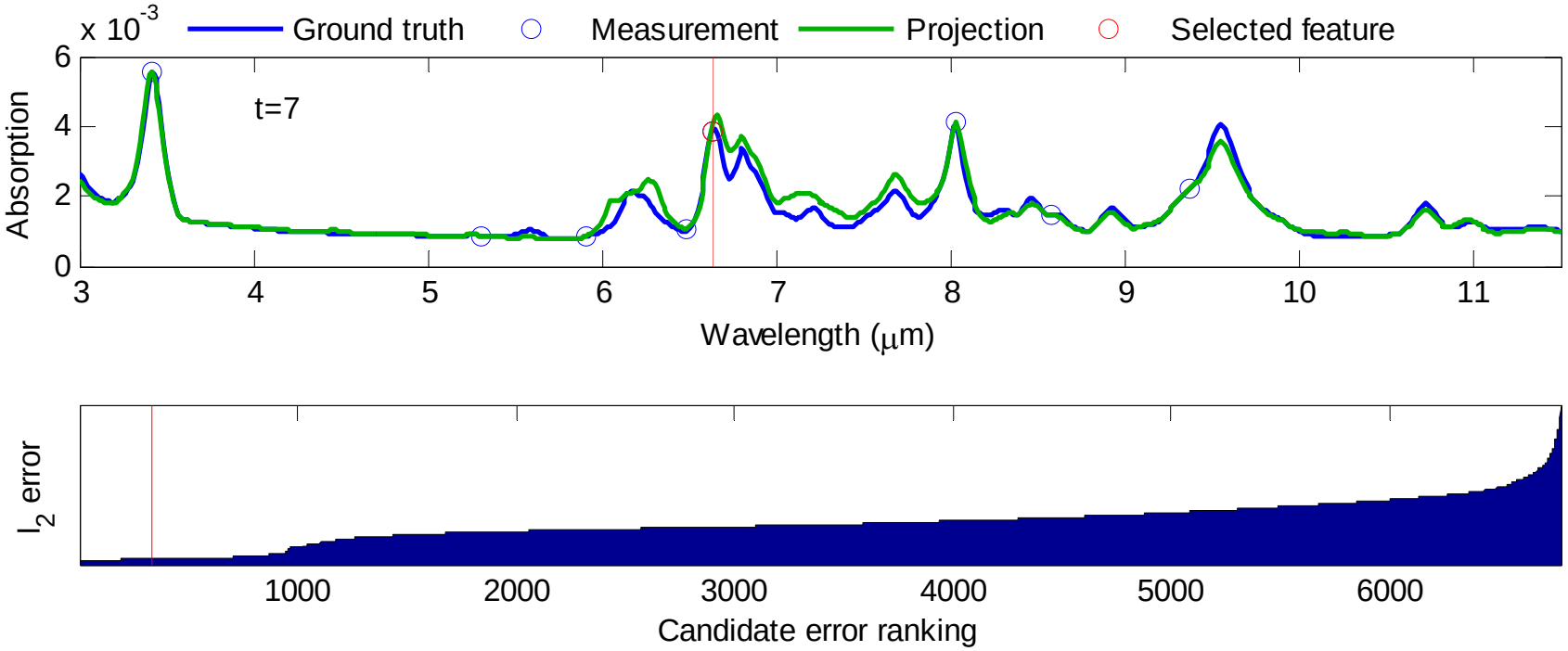
Step 5


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=5
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

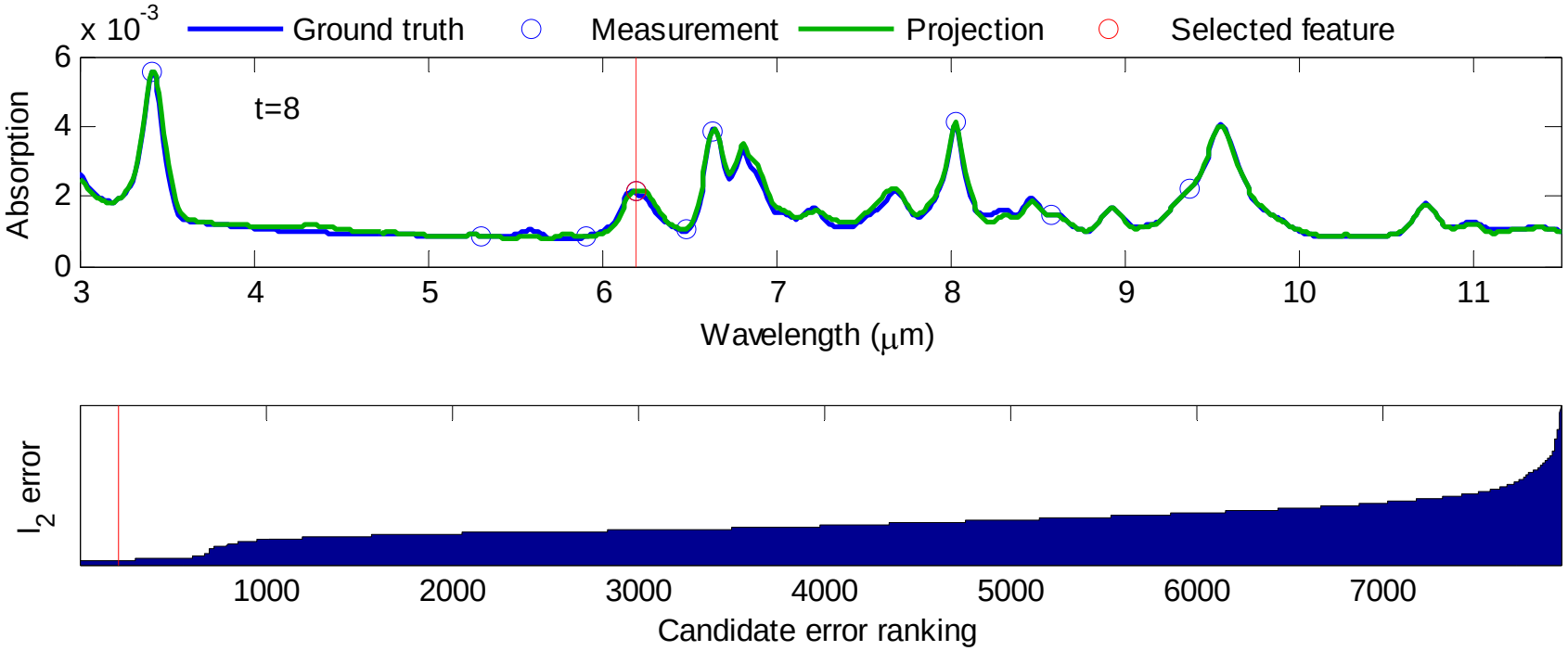
Step 6


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=6
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

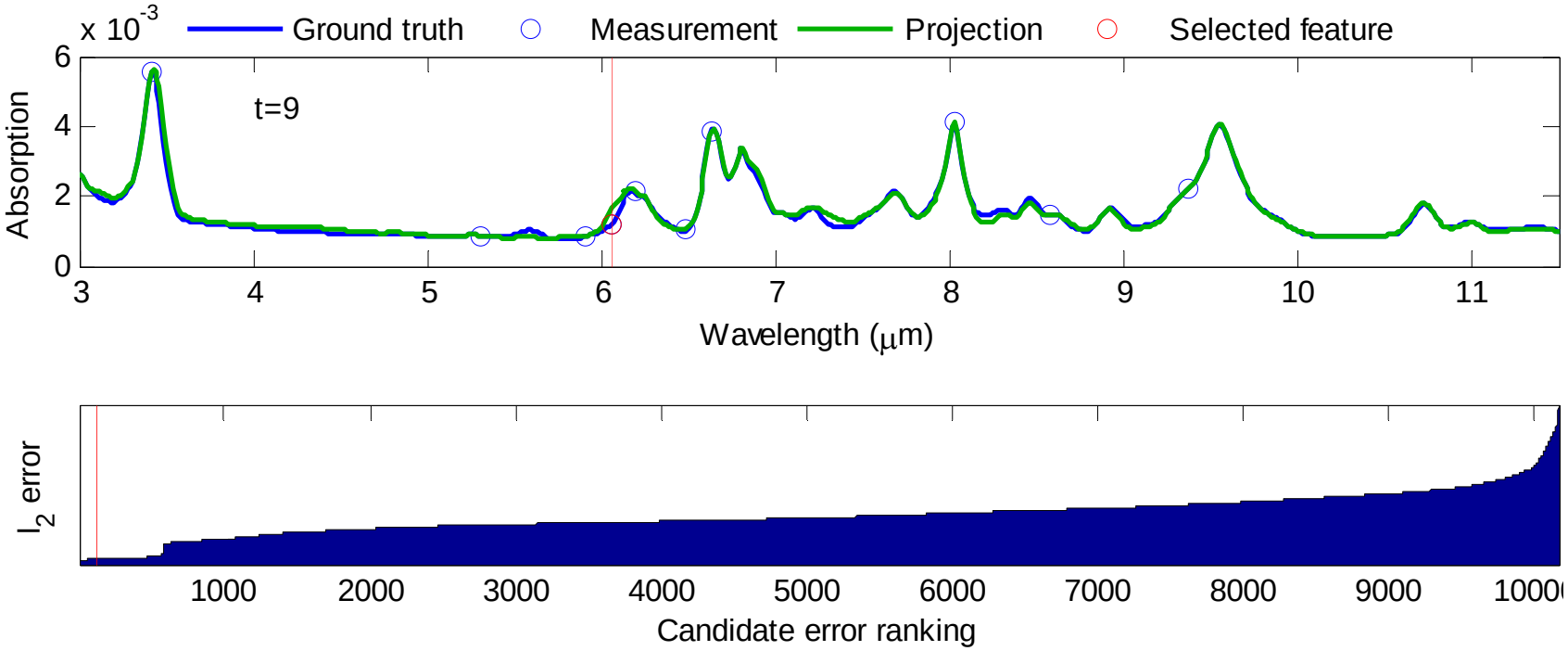
Step 7


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=7
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

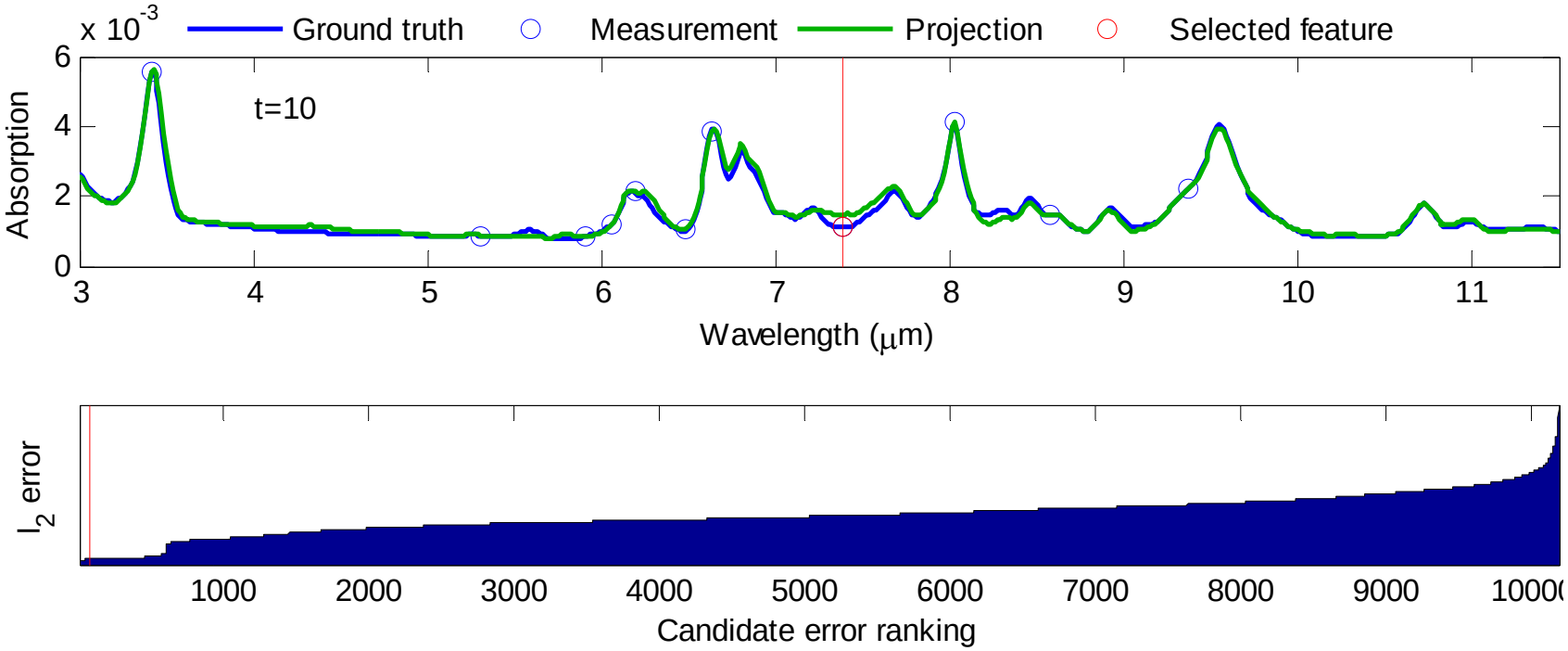
Step 8


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=8
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

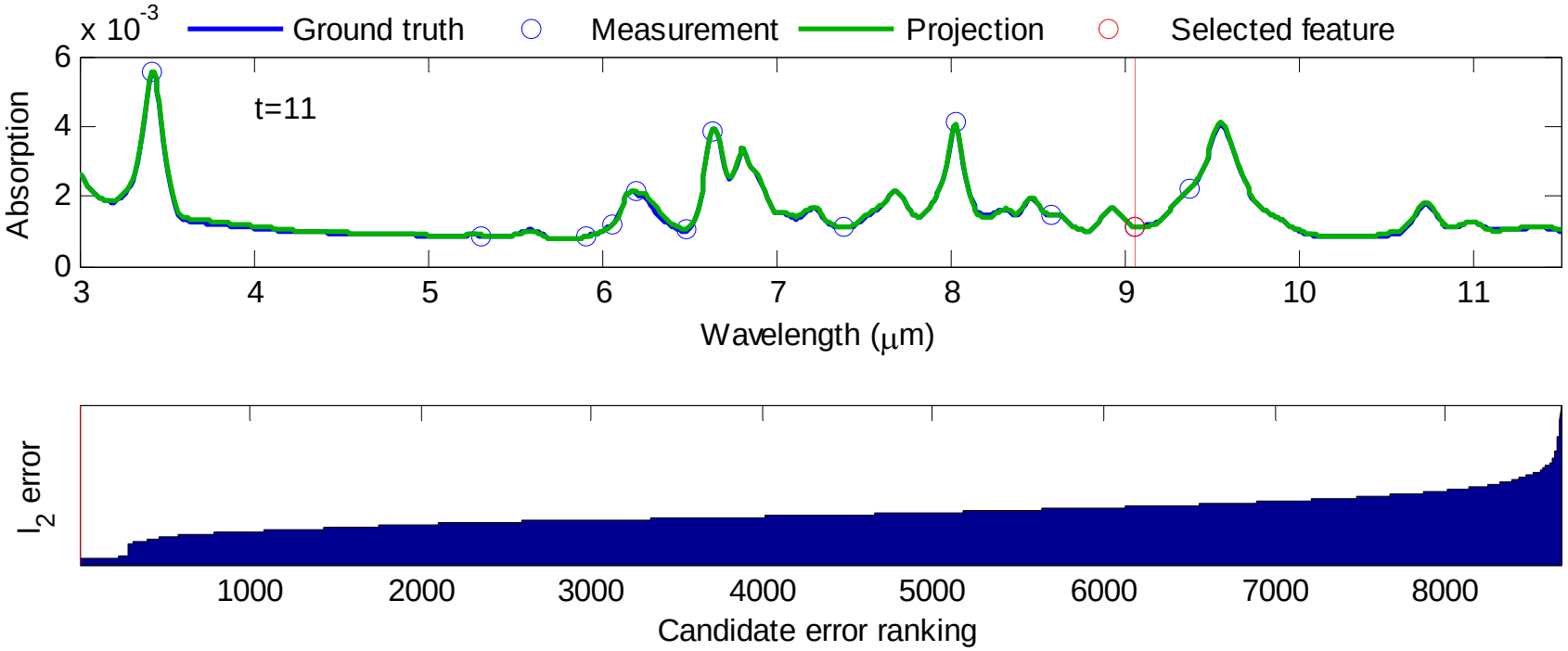
Step 9


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=9
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

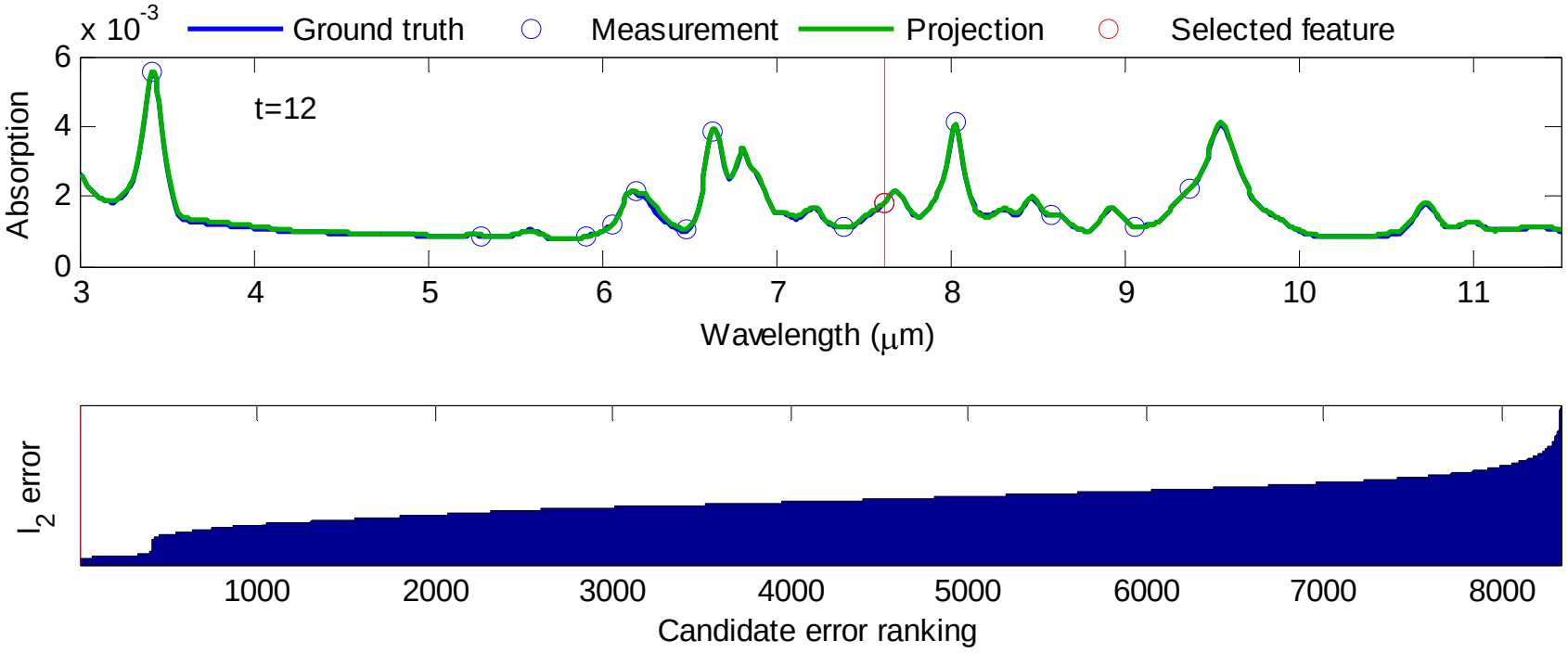
Step 10


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=10
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

Step 11


x 10^-3
Ground truth
Measurement
Projection
Selected feature
t=11
Absorption
Wavelength (μm)
l2 error
Candidate error ranking

Step 12



Converged

Overall performance

Baseline: passive sensing

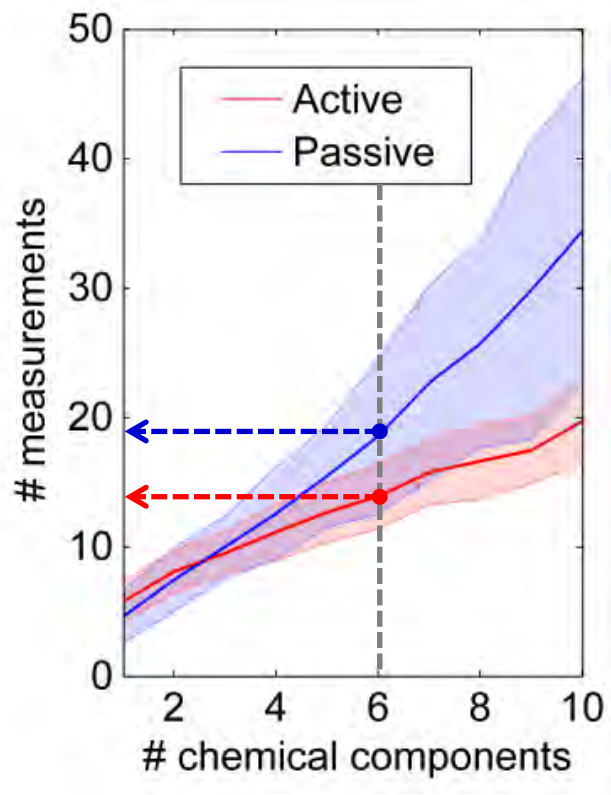
- Sequential forward feature selection
- Trained to distinguish all 100 chemicals
- Generates a fixed sequence of wavelengths

Experimental protocol

- Randomly pick chemicals and assign random concentrations
  - Concentration has to be significant (larger than 10%)
- Mixtures have from 1 up to 10 chemical components
- Stopping criteria: same l_2 error threshold for both methods

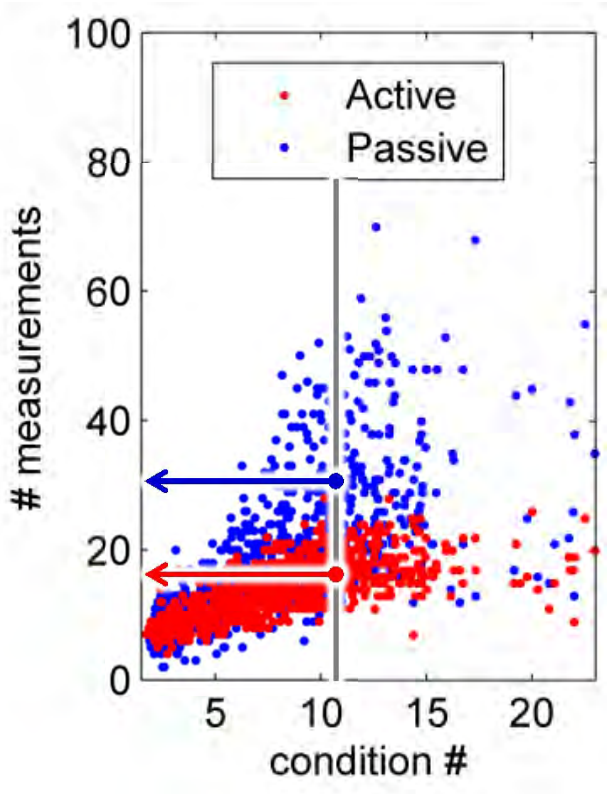
Number of measurements needed

- Fewer measurements means cost savings
- For each # components we ran 100 examples



Stability of the solution

- Measured with the condition number of A'
  - A measure of correlation among wavenumbers
- Higher condition # ⇒ higher correlation ⇒ less stability



Discussion and future work

Discussion

- Multimodal search provides alternative candidates, which help tackle ill-posed problems
- Only a small fraction of candidate solutions are needed to reveal the uncertainty (by virtue of the back-projection)

Future work

- Experimental validation on real FPI sensor
- Improvements to the algorithm
  - Encouraging diversity to the candidate pool
  - Over-fitting criteria for trace analysis

Thank you
Questions?