# Understanding fused sensor system capabilities and limitations


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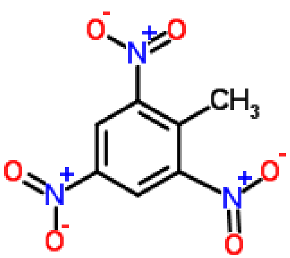
# Summary

Fusion of multiple sensors expands the measurement space of a detection system, and thus provides the potential for enhanced sensing capabilities.

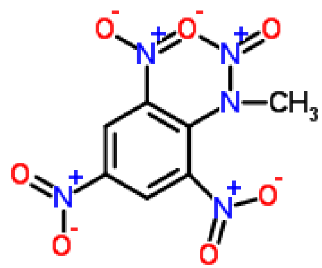
However, such enhancement is not guaranteed, and it is important to keep in mind that selectivity of multisensor systems is highly context-dependant.

It is possible to estimate best case fused system potential performance gains through an understanding of the performance characteristics of component sensor systems.

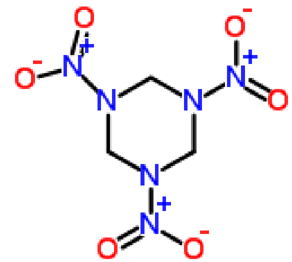
# Target Analytes



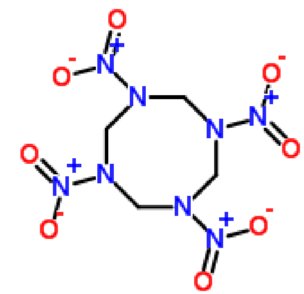
TNT



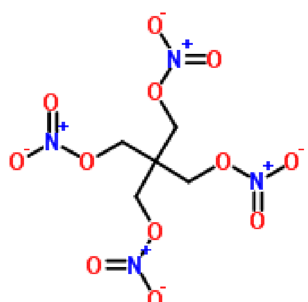
Tetryl



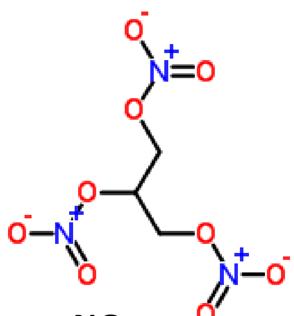
RDX



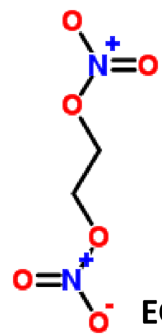
HMX



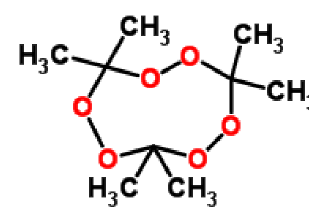
PETN



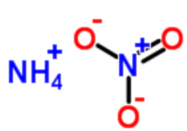
NG



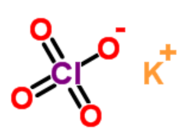
EGDN



TATP



Ammonium Nitrate



Potassium Perchlorate

# Analyte Properties

| | | arom | $NO_2$ | -N- | $NO_3$ ester | -O-O- | salt | VP /atm | MP C | MW |
|---|---|---|---|---|---|---|---|---|---|---|
| Low volatility | TNT | x | x3 | | | | | $10^{-9}$ | 80.35 | 227.13 |
| | Tetryl | x | x4 | x1 | | | | $10^{-13}$ | 129.5 | 287.15 |
| | RDX | | x3 | x3 | | | | $10^{-11}$ | 205.5 | 222.12 |
| | HMX | | x4 | x4 | | | | $10^{-14}$ | 276 | 296.16 |
| | PETN | | | | x4 | | | $10^{-11}$ | 141.3 | 316.14 |
| Semi-Volatile | NG | | | | x3 | | | $10^{-6}$ | 14 | 227.09 |
| | EGDN | | | | x2 | | | $10^{-5}$ | -22 | 152.1 |
| | TATP | | | | | x3 | | $10^{-6}$ | 91 | 222.2 |
| Salts | $NH_4NO_3$ | | | | | | x | $10^{-8}$ | 169.6 | 80.052 |
| | $KClO_4$ | | | | | | x | - | 525 | 138.55 |

# Motivation for Multisensor Approach

To leverage unique sources of information from multiple sensing modalities to provide more accurate assessment than possible with single sensors.

- Reduction of false positives (**enhanced selectivity**)
- Improved detection of target analytes (**enhanced sensitivity**)
- Capability to detect a **wider range of target analytes**

# "Unique sources" of information

**1) Sensors that detect different target analytes**

**2) Sensors that detect the same analytes, but with…**

- Different performance characteristics
- Different statistical properties
- Different output data format/ sensing modality

***Fused systems consisting entirely of COTS explosive detectors***

**3) Sensors that provide information that aides in target analyte assessment (but do not directly identify it)**

- Detects potential interferant compounds for another sensor
- Classifies target analyte as separate from other compounds
- Provides meta information about performance of other sensors

***Fused systems with context-dependant, non target-specific sensors***

# Current Landscape

FirstDefender RM
(Thermo Scientific)

Hazmat ID Ranger
(Smiths Detection)

Quantum Sniffer QS-H150
(Implant Sciences Corp.)

Fido Verdict (ICx Technologies)

TrueDefender FT/FTG
(Thermo Scientific)

MobileTrace
(Morpho Detection)

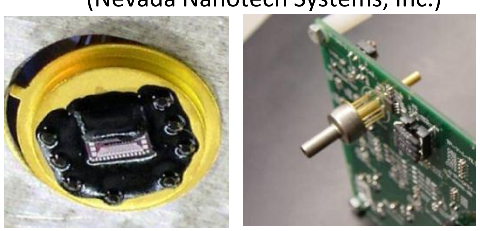
Multi-Mode Threat Detector
(Smiths Detection)

EVD 3000+
(Scintrex)

E3500 Chemilux
(Scintrex)


Fido PaxPoint (ICx Technologies)

NevadaNano Self Sensing Array
(Nevada Nanotech Systems, Inc.)



zNose Model 4500
(Electric Sensor Technology)

# Current Landscape

## Spectrometric

IMS: molecular size and shape
MS: molecular size, fragmentation

## Spectroscopic

FTIR: vibrational structure
Raman: vibrational, rotational structure

## Chemical Adsorption

Surface Acoustic Wave (SAW)
Micro cantilever (MEMS)

## Chemical Reactivity

Electrochemical sensors
Fluorescence Quenching
Chemical Luminescence
Colormetric sensors

# Sensor Modalities

Binary-valued output (detect vs no detect)

Continuously valued scalar output (absorbance at one λ)

Vector output (spectrum)

**Measurement space of the fused system is the outer product of the output space of each component.**

# Multisensor System Design

## What are the requirements?

target compounds
potential interferants
operating conditions

## What sensors will be used?

multiple COTS detection technologies
augment one or more COTS systems with additional sensors
new sensors, purpose built for fused data systems

## How will an output decision be derived from data?

# Detection and Decision Theory

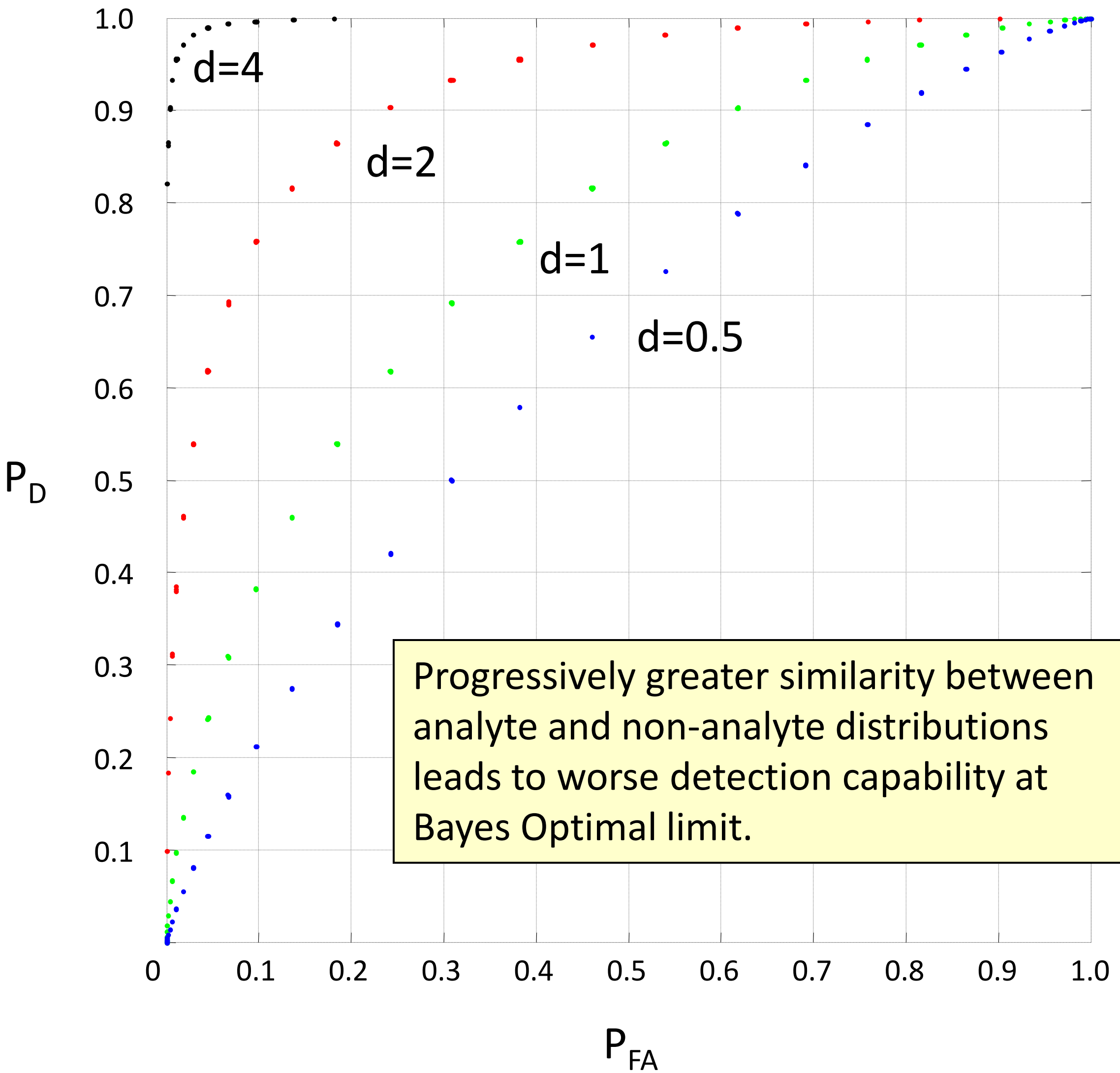
Detection of an analyte is a decision that is made on the basis of measured sensor data.

Decision theory: arrive at an optimal decision, given observable evidence and knowledge of the statistical distributions.

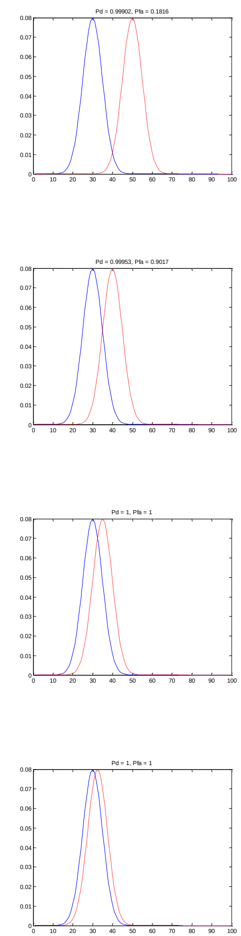
Ability of a sensor (or multisensor system) to detect an analyte rests on the distribution of sensor responses observed when the analyte is present and when it is not.

Adding or removing sensors, incorporating other compounds and interferences, and varying the amount of each present will alter these distributions, leading to changes in the system's detection ability.

# ROC curves



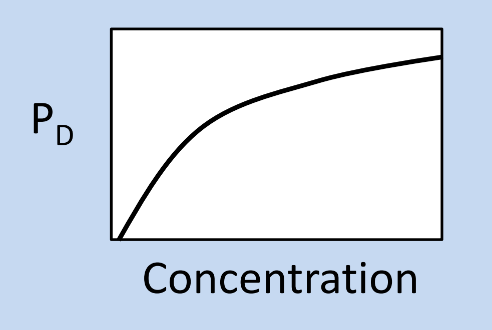

Progressively greater similarity between analyte and non-analyte distributions leads to worse detection capability at Bayes Optimal limit.




$$d = \frac{\Delta\mu}{\sigma}$$

# System Performance Measures

**Sensitivity** – reflected in the functional dependence of $P_D$ with analyte concentration




**Selectivity** – the statistical independence (or lack thereof) of sensor response in the presence of non-analyte species (interferants)

| | |
|---|---|
| *Full Selectivity* | P(**Detect**\|Interferant) = P(**Detect**) |
| *Partial Selectivity* | P(**Detect**\|Interferant) ≠ P(**Detect**) |
| *Non-Selective* | P(**Detect**\|Interferant) = P(**Detect**\|Analyte) |

***How do individual sensor performance characteristics contribute to overall fused system performance?***

# Multisensor Detection

A fused system can be visualized as a series of measurements made on the same sample

This system has a characteristic measurement space that contains every possible collection of sensor responses that the system can generate

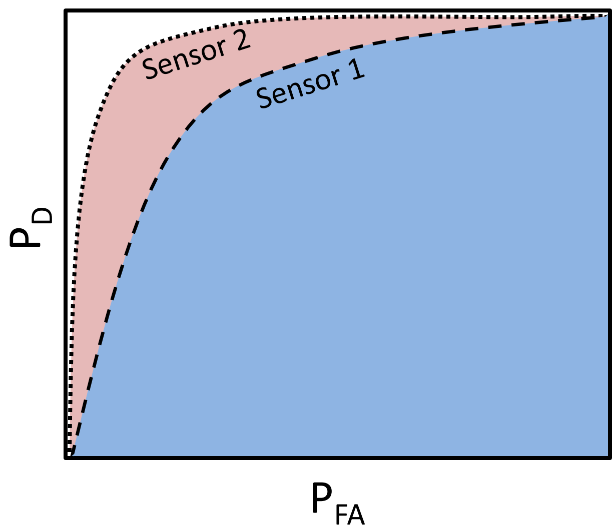
Conditional probability distributions in this space describe the system's response to analytes, interferants, etc.

The separability of these distributions indicates how difficult the detection challenge will be.  (Bayes Optimal classifier provides best possible performance)

# Measuring Selectivity

## Area Under ROC (AUC)

ROC summarizes tradeoff between $P_D$ and $P_{FA}$ for a give sensor. Area under the ROC varies between 0.5 and 1

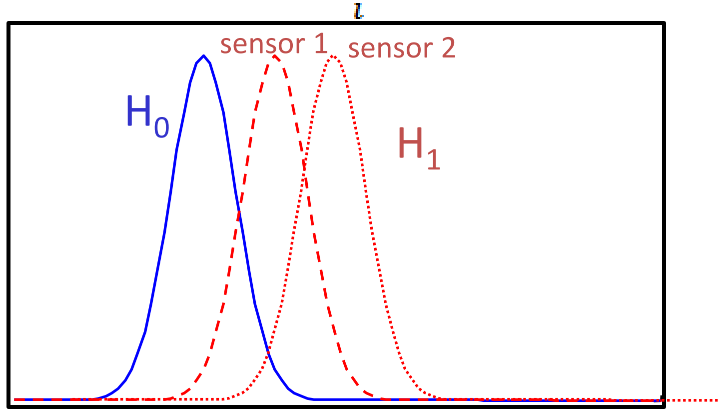



Coin Flip | 0.5 < Sensor 1 AUC < Sensor 2 AUC < 1 | Perfect Detection

## KL Divergence

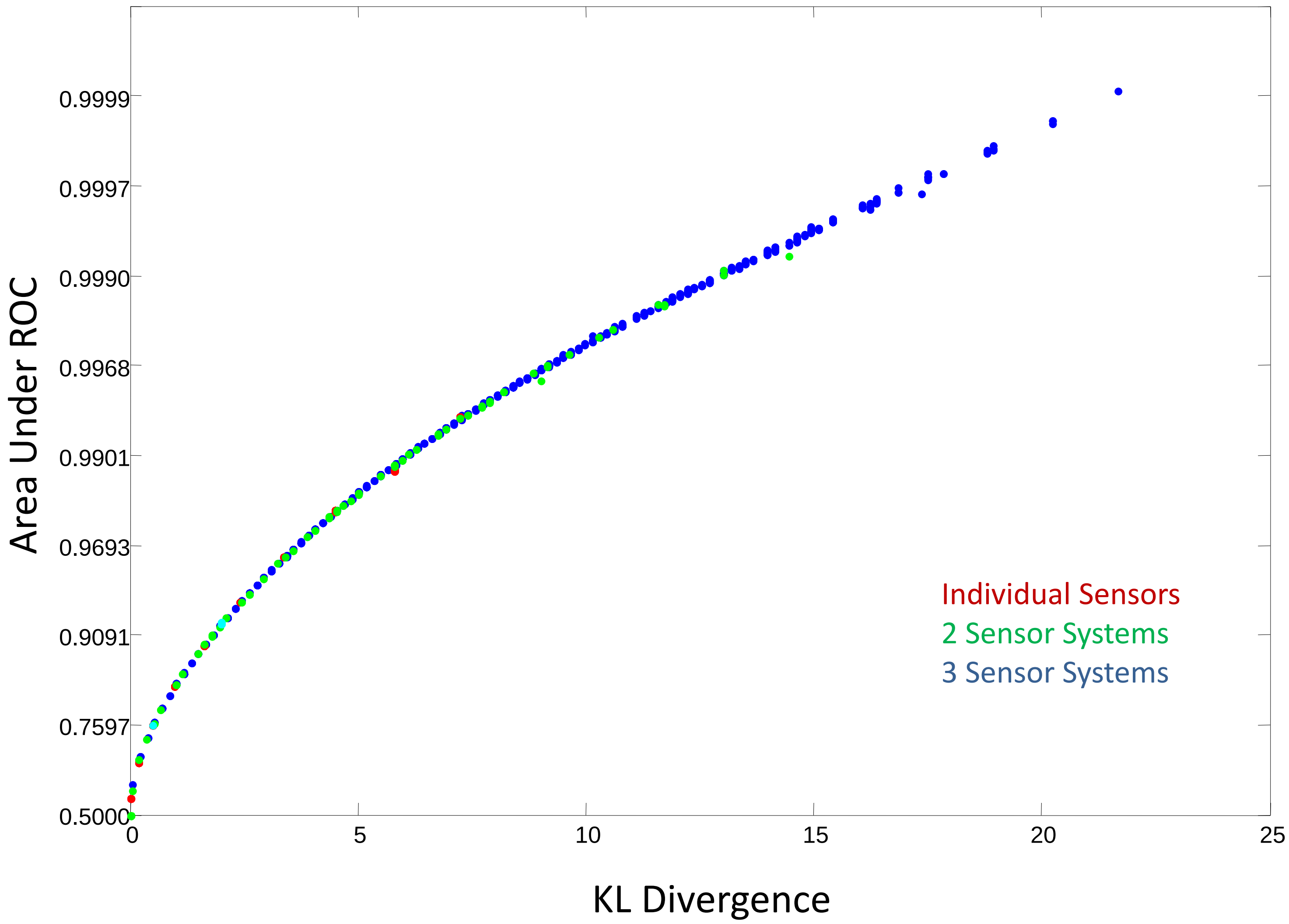
KL Divergence provides a measure of the difference between two probability distributions, $H_1$ and $H_0$

$$D_{KL}(H_1 \parallel H_0) = \sum_i H_1(i) ln \frac{H_1(i)}{H_0(i)}$$



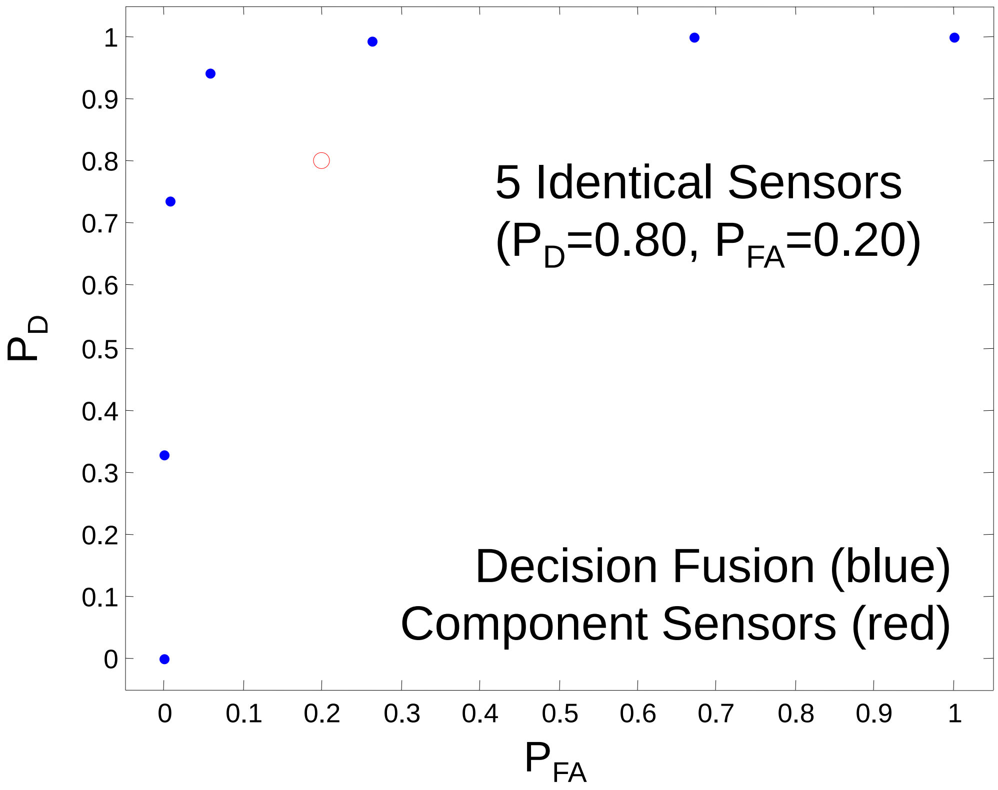

Complete Overlap | 0 < Sensor 1 $D_{KL}$ < Sensor 2 $D_{KL}$

# KL Divergence vs Area Under ROC



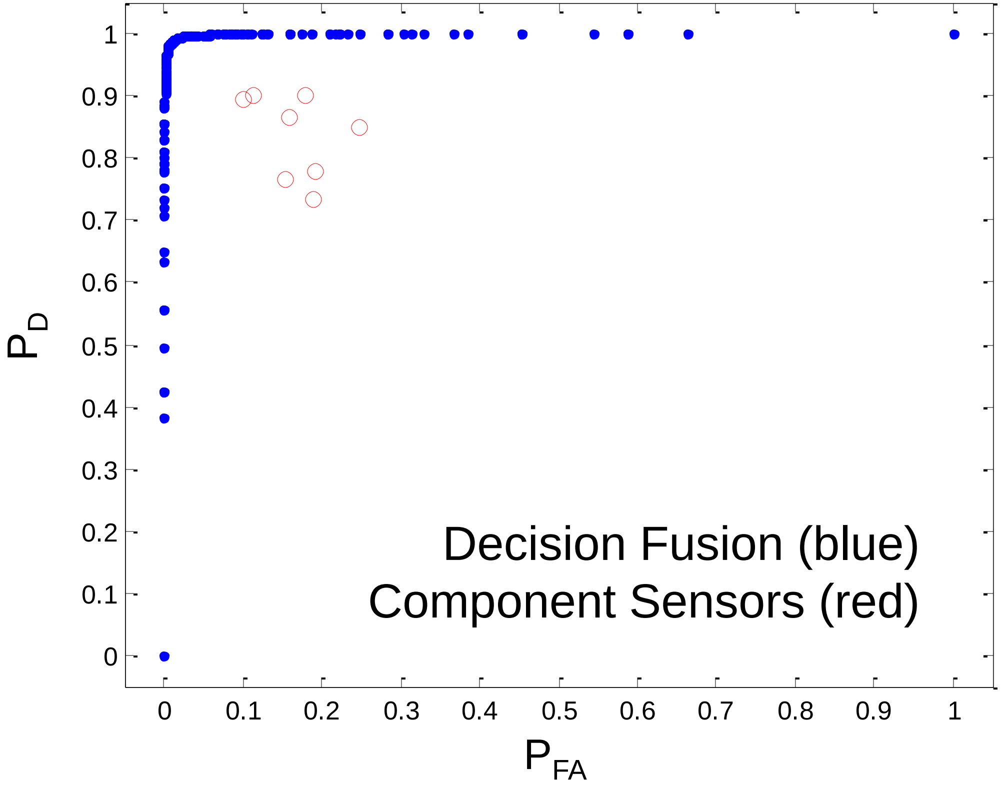
# Example: “Black Box” Binary Sensors

Suppose one has a collection of binary output sensors with known, fixed probabilities of detection and false alarm.



# Example: "Black Box" Binary Sensors

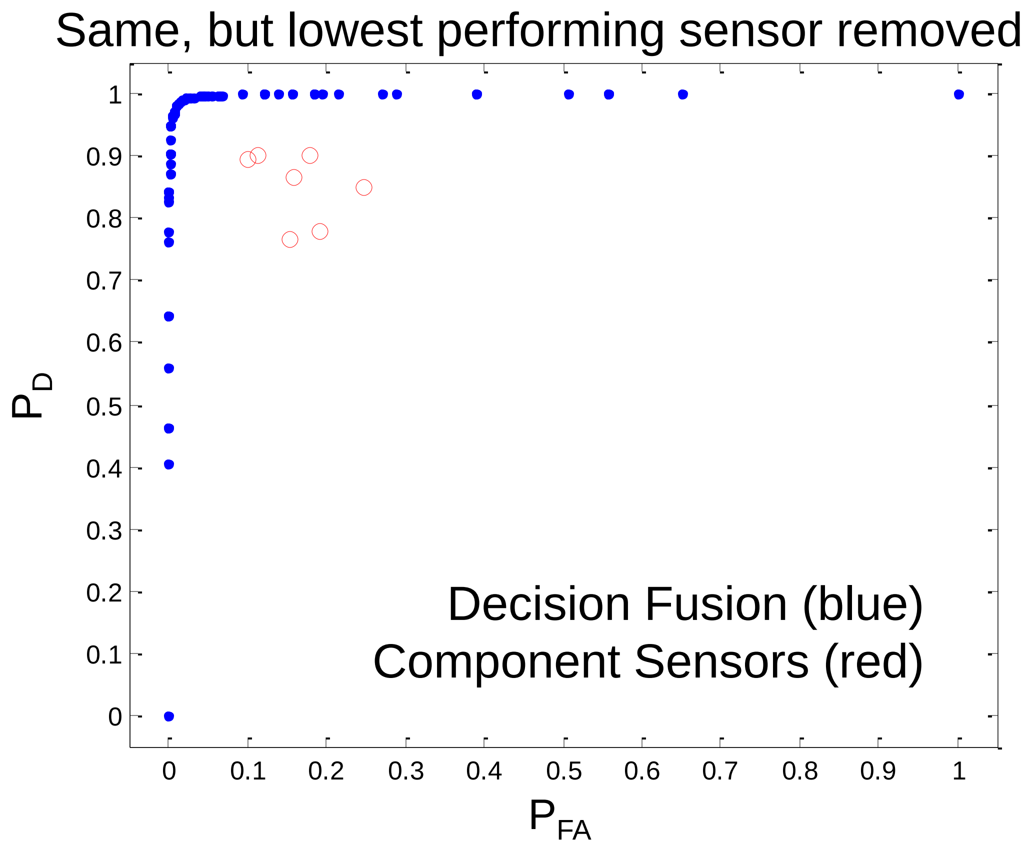
8 component sensors, random $P_D$ and $P_{FA}$ values




$0.7 < P_D < 0.9$
$0.1 < P_{FA} < 0.3$

ROC curve for a fused sensor system with eight component sensors with random $P_D$ and $P_{FA}$ values. Dots represent possible performance regimes for the fused system. The circles depict the $P_D$ and $P_{FA}$ values associated with each of the eight component sensors.

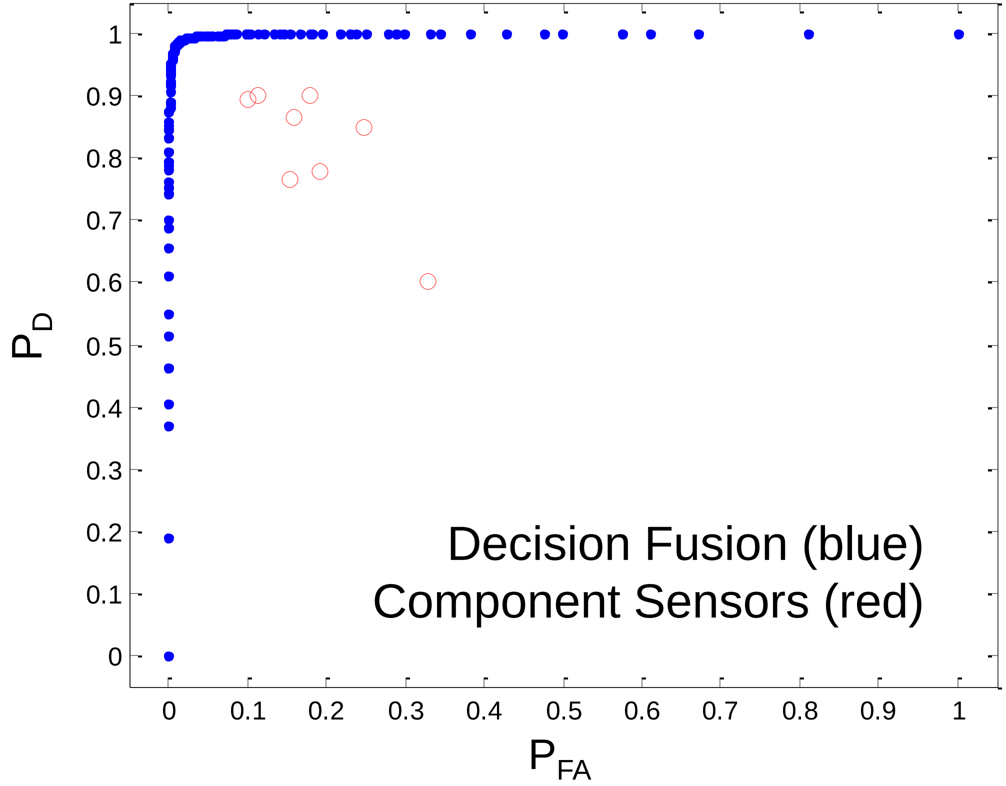
# Example: “Black Box” Binary Sensors




ROC curve for the fused sensor system shown in Figure 4, with one low-performing sensor removed.

# Example: “Black Box” Binary Sensors

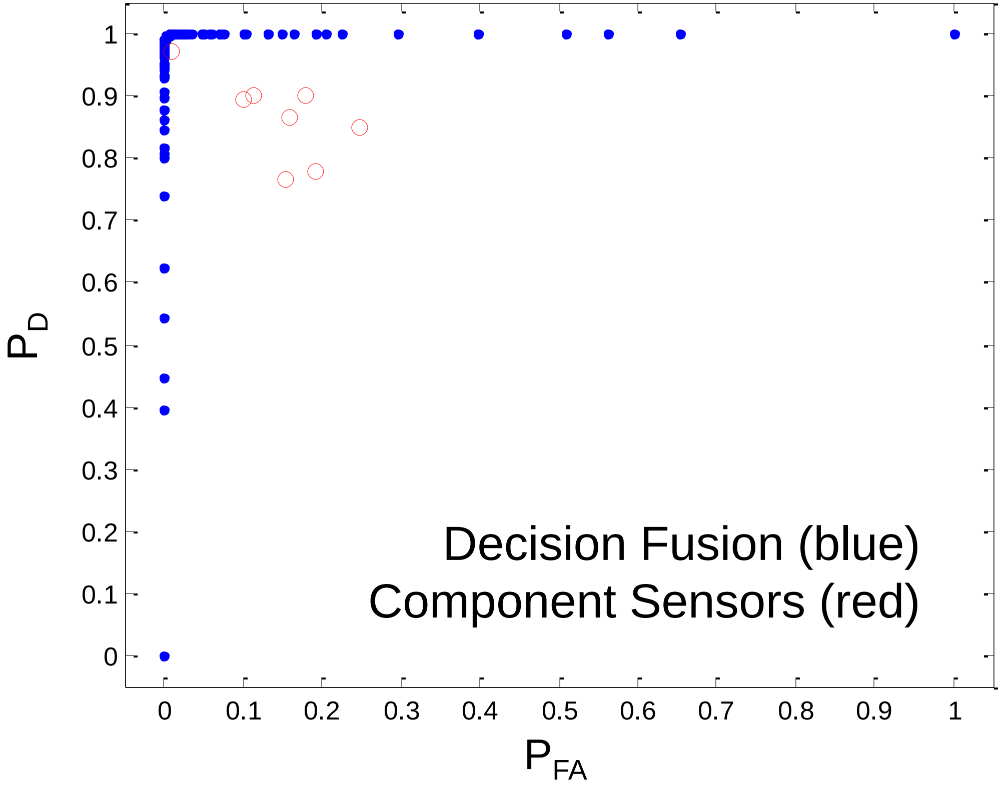
Same 7 sensors, add low performing sensor $P_D$=0.6 and $P_{FA}$=0.33




ROC curve for the fused sensor system shown in Figure 5, with one lower-performing sensor added in with $P_D$=0.6 and $P_{FA}$=0.33.

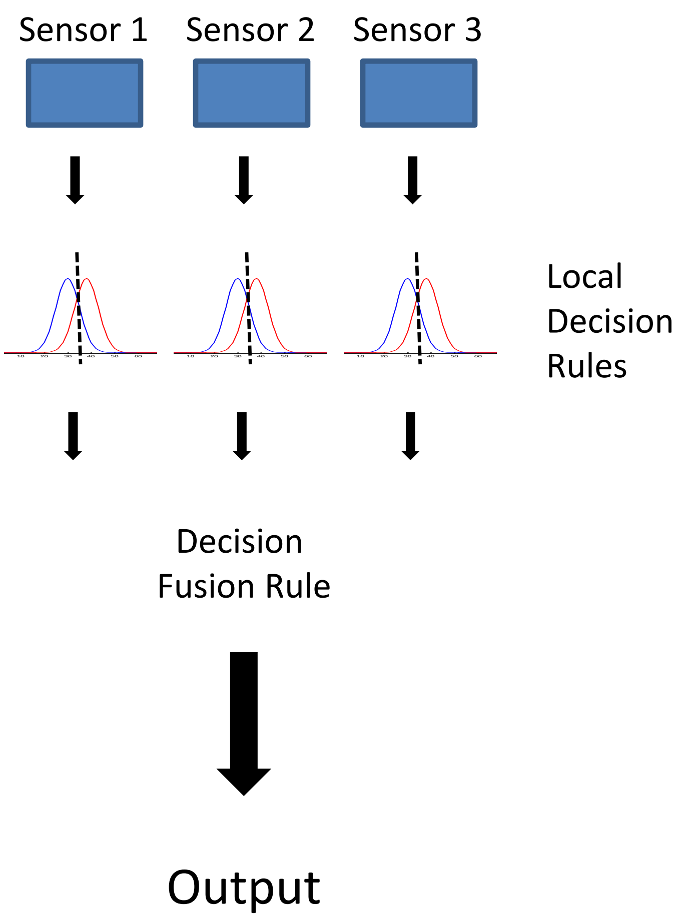
# Example: "Black Box" Binary Sensors

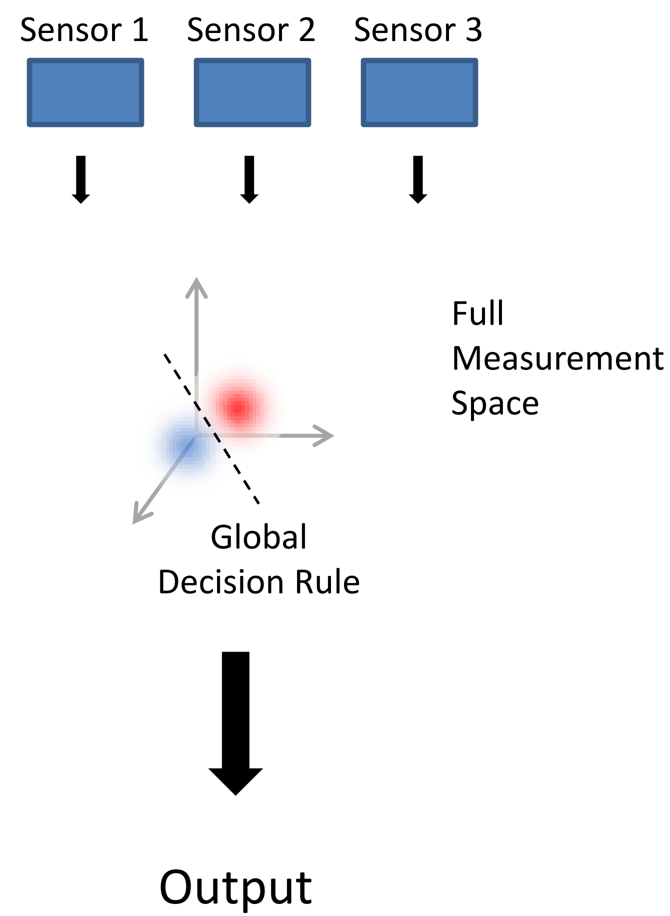
Same 7 sensors, add high performing sensor $P_D$=0.97 and $P_{FA}$=0.01




ROC curve for the fused sensor system shown in Figure 5, with one higher-performing sensor added in with $P_D$=0.97 and $P_{FA}$=0.01.

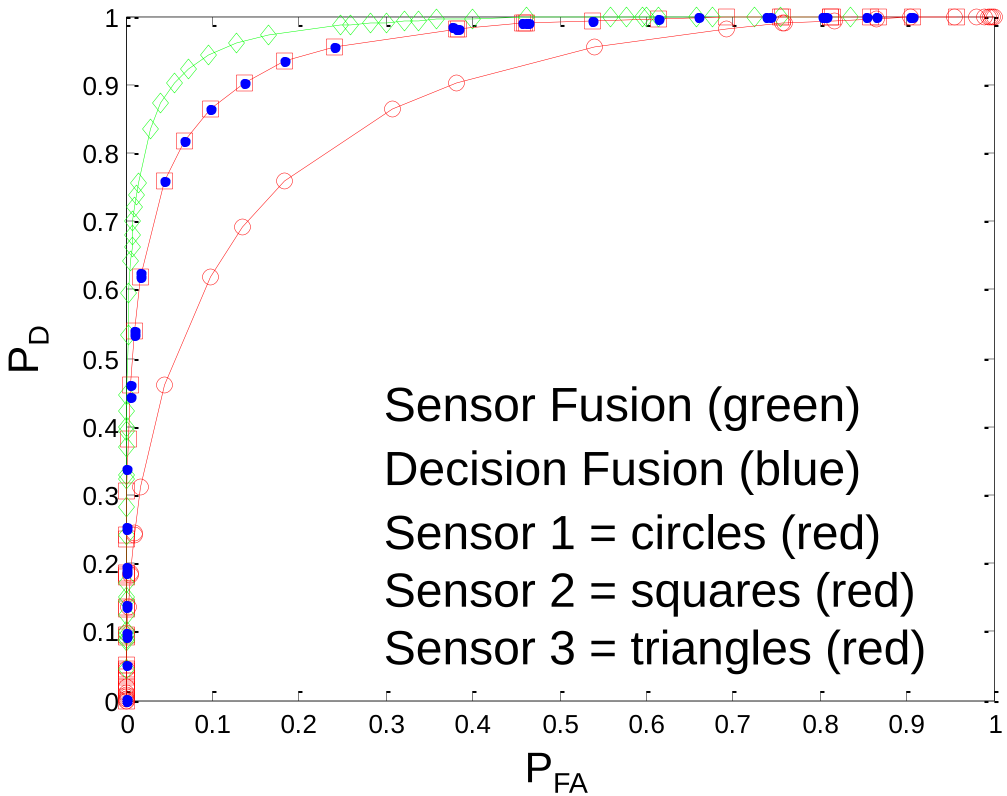
# Example: Binary vs. Univariate Sensors



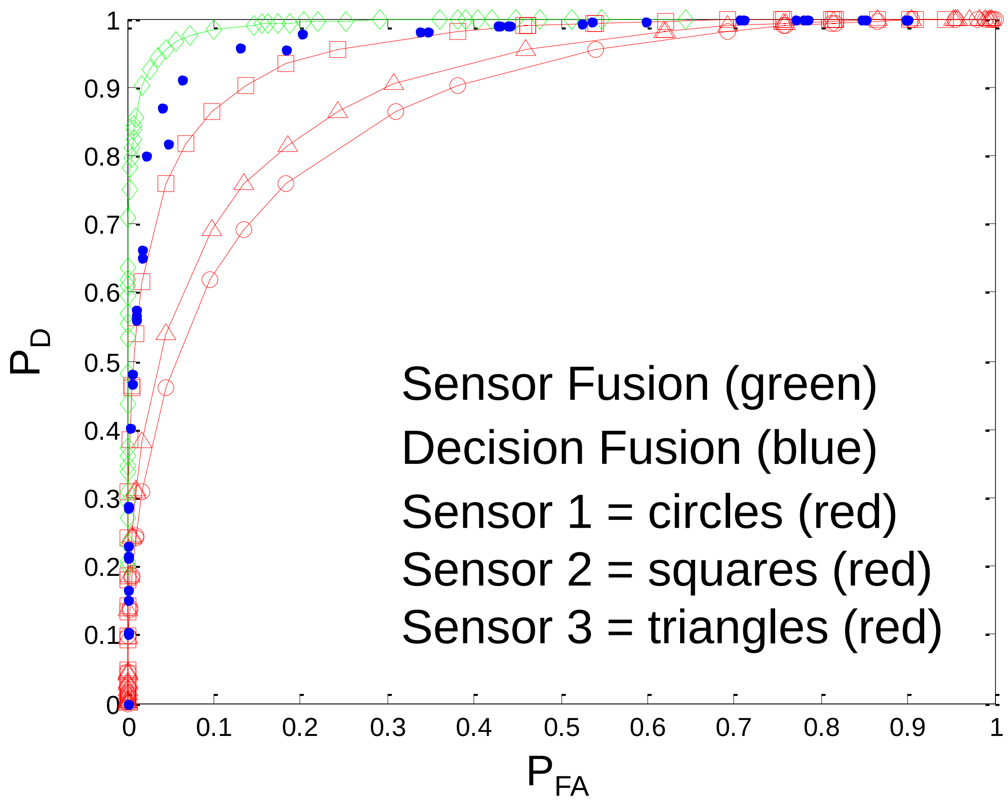
# Example: Binary vs. Univariate Sensors

ROC curves for a fused sensor system with two component univariate sensors.

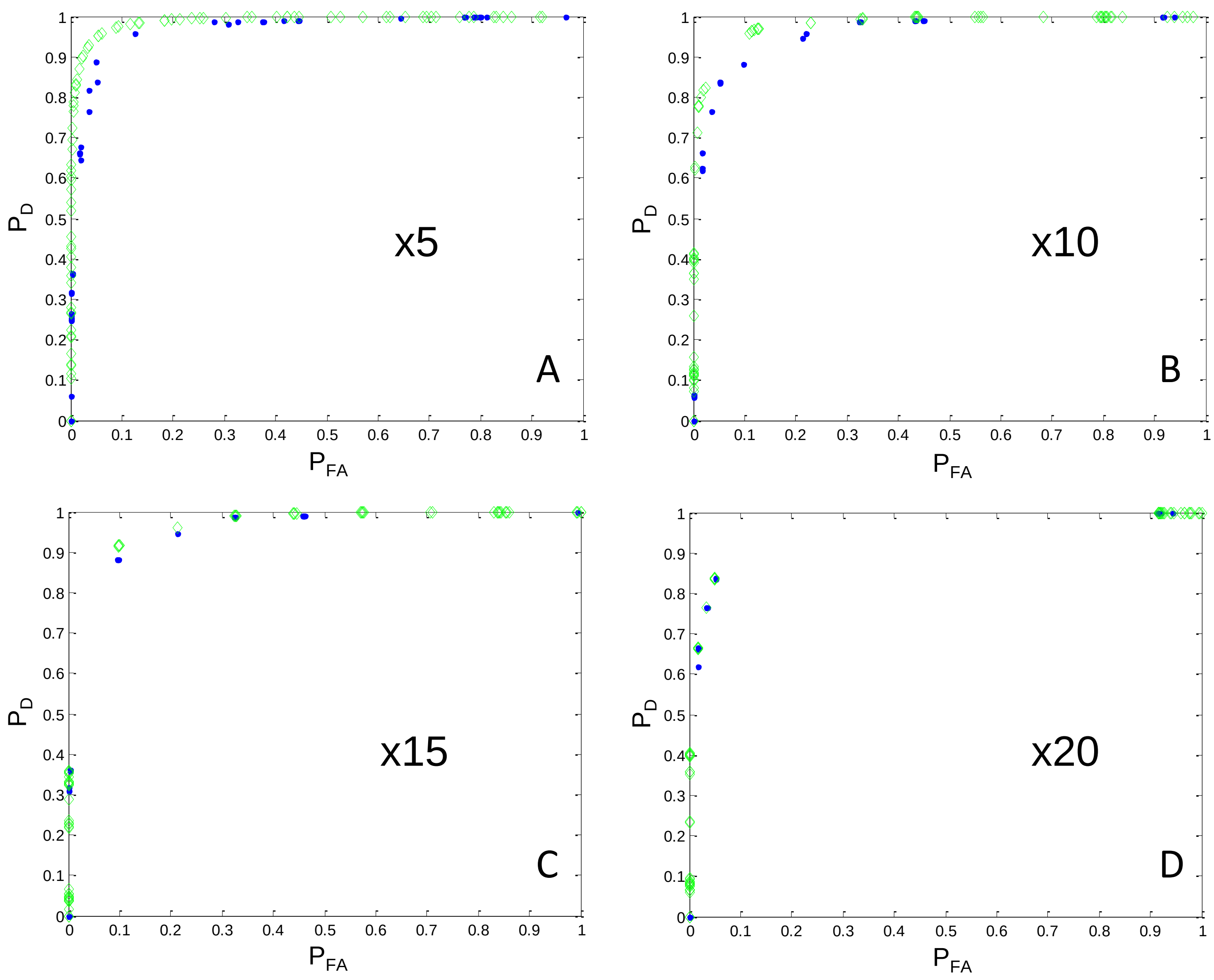


# Example: Binary vs. Univariate Sensors

ROC curves for a fused sensor system with three component sensors.



# Example: Binary vs. Univariate Sensors



# Example: Partially Selective Arrays

Consider a hypothetical array of 5 sensors and 5 potential analytes

Analyte concentrations

| analyte | conc. | relative response factors | | | | |
|---|---|---|---|---|---|---|
| 1 | 1 | 0.97 | 0.27 | 0.14 | 0.91 | 0.77 |
| 2 | 1 | 0.87 | 0.02 | 0.64 | 0.16 | 0.23 |
| 3 | 1 | 0.25 | 0.21 | 0.54 | 0.31 | 0.61 |
| 4 | 1 | 0.92 | 0.52 | 0.53 | 0.40 | 0.82 |
| 5 | 1 | 0.63 | 0.88 | 0.35 | 0.25 | 0.46 |

Captures the fundamental selectivity of sensor array

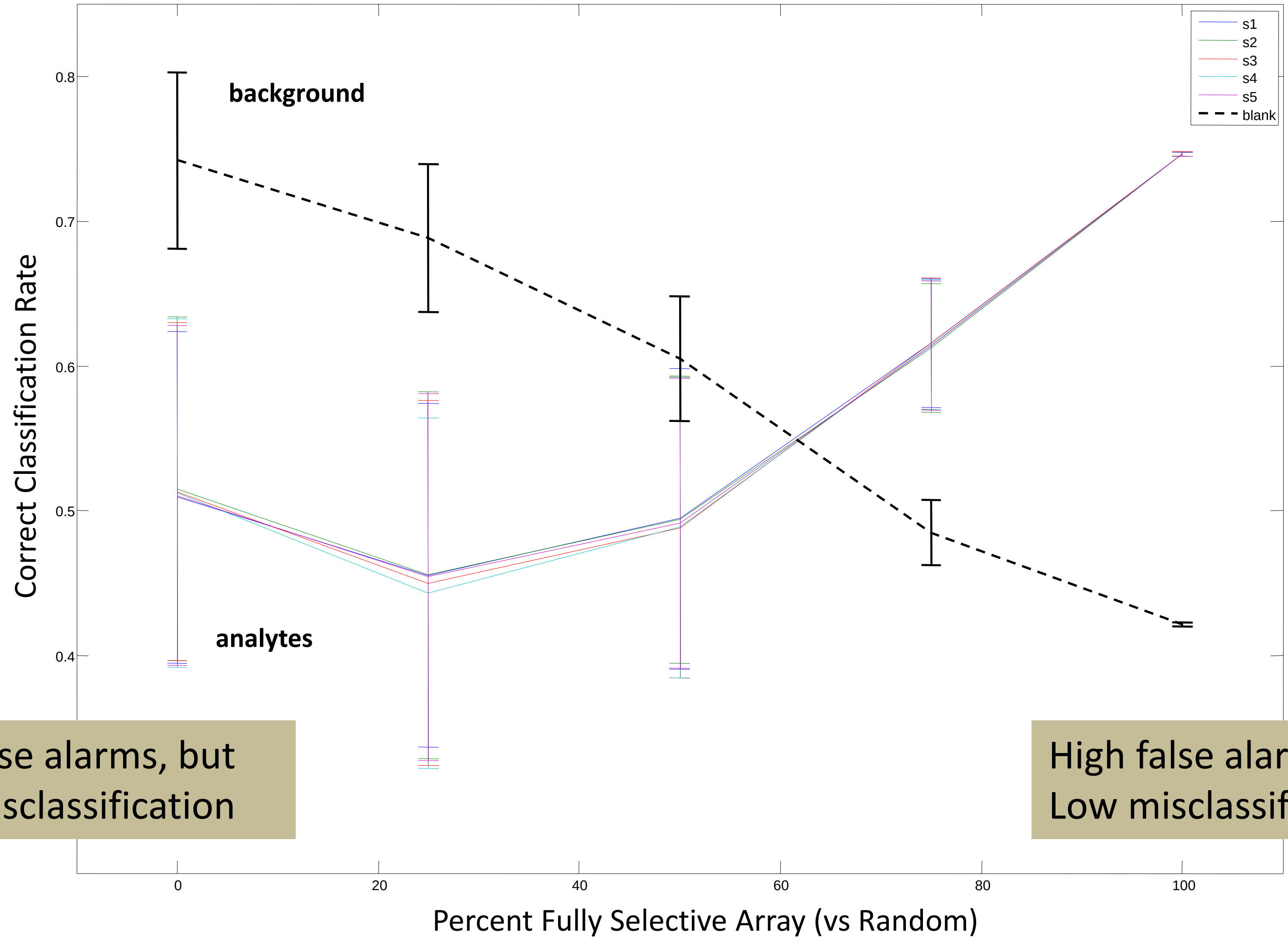
| | | | | | |
|---|---|---|---|---|---|
| ref. response factor | 5 | 5 | 5 | 5 | 5 |
| measurement error | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 |
| background signal | 0 | 0 | 0 | 0 | 0 |
| sensor number | 1 | 2 | 3 | 4 | 5 |

← Sensor sensitivities

← Sensor measurement error

← Sensor background response

# Example: Partially Selective Arrays



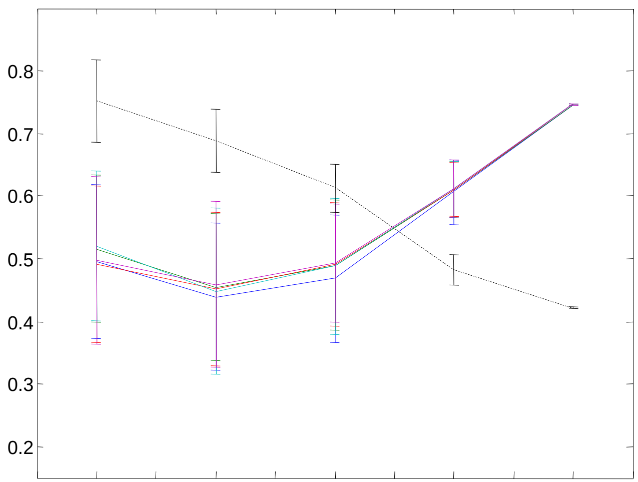

Low false alarms, but high misclassification

High false alarms, but Low misclassification

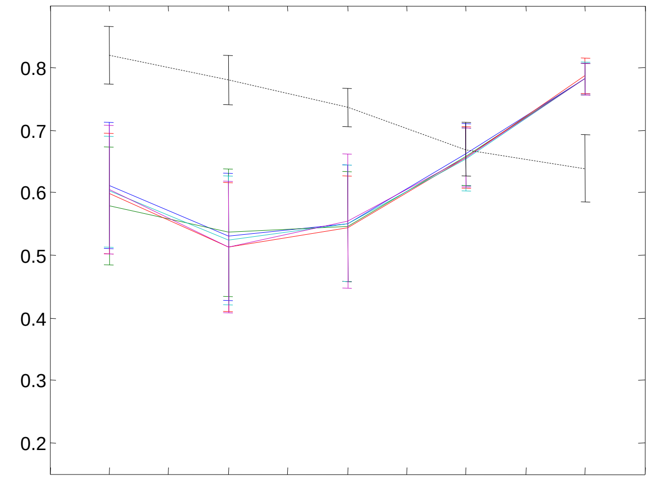
# Example: Partially Selective Arrays

Overdetermined, k > n

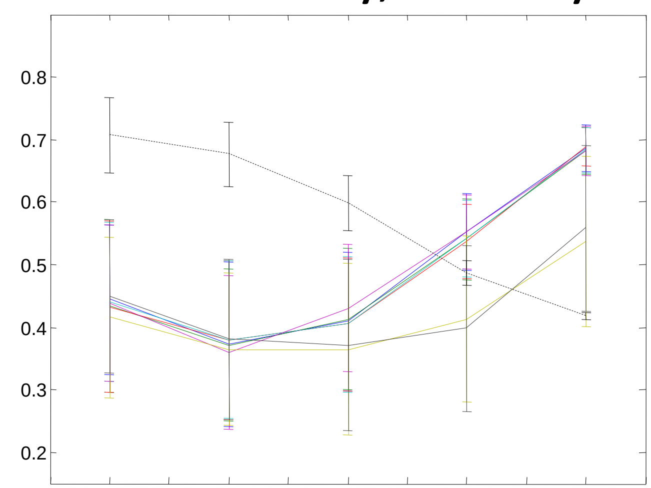
5 sensor array, 5 analytes




7 sensor array, 5 analytes




5 sensor array, 7 analytes




Underdetermined, k < n

# System Design Considerations

Define the scope of the sensing scenario

Individual sensor performance characteristics

Sensor modality, local data processing steps

Sensor response distribution estimates

Modes of interference

# Summary

Fusion of multiple sensors expands the measurement space of a detection system, and thus provides the potential for enhanced sensing capabilities.

However, such enhancement is not guaranteed, and it is important to keep in mind that selectivity of multisensor systems is highly context-dependant.

It is possible to estimate best case fused system potential performance gains through an understanding of the performance characteristics of component sensor systems.

# Acknowledgements

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# Backup Slides

# Implications of Multisensor Approach

**Adding sensors increases the size of the measurement space**

This provides the potential for greater separability between analytes, as well as detection of a wider range of analytes

BUT

Estimation of conditional probability distributions rapidly becomes more complicated as the dimensionality increases

# Identifying Compounds

## Spectrometric

IMS:  molecular size and shape
MS: molecular size, fragmentation


Quantum Sniffer QS-H150
(Implant Sciences Corp.)


MobileTrace
(Morpho Detection)

Multi-Mode Threat Detector
(Smiths Detection)

IMS is the current leader in explosives detection technology, demonstrating sensitive detection of multiple analytes.

Can be prone to high false alarm rates due to interferants.

MS has the potential to be highly selective and sensitive, but is difficult to make portable and retain high performance.

# Identifying Compounds

FirstDefender RM
(Thermo Scientific)

Hazmat ID Ranger
(Smiths Detection)

## Spectroscopic

FTIR:  vibrational structure

Raman: vibrational, rotational structure

Fido Verdict (ICx Technologies)

TrueDefender FT/FTG
(Thermo Scientific)

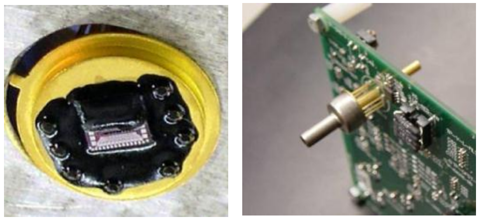
Spectral information lends potentially high selectivity for multiple analytes, but devices generally suffer from low detection limits.

# Identifying Compounds

Selectivity dictated by specificity of the interaction between the sensor and the analyte. Could require multiple devices for detection of a wide range of analytes. Miniaturized sensing elements suggest potential for incorporation in portable devices

## Chemical Adsorption

Surface Acoustic Wave (SAW)
Micro cantilever (MEMS)



NevadaNano Self Sensing Array
(Nevada Nanotech Systems, Inc.)

zNose Model 4500
(Electric Sensor Technology)

# Identifying Compounds

Generally tailored to a specific class of compound, rather than multiple analyte classes, can be prone to drift or difficult interpretation of results.  Multiple sensors would be required for a wide range of analytes, but a limited number could be useful as a means to augment multi-analyte detectors to improve false alarm rates.

EVD 3000+
(Scintrex)

E3500 Chemilux
(Scintrex)

Fido PaxPoint (ICx Technologies)

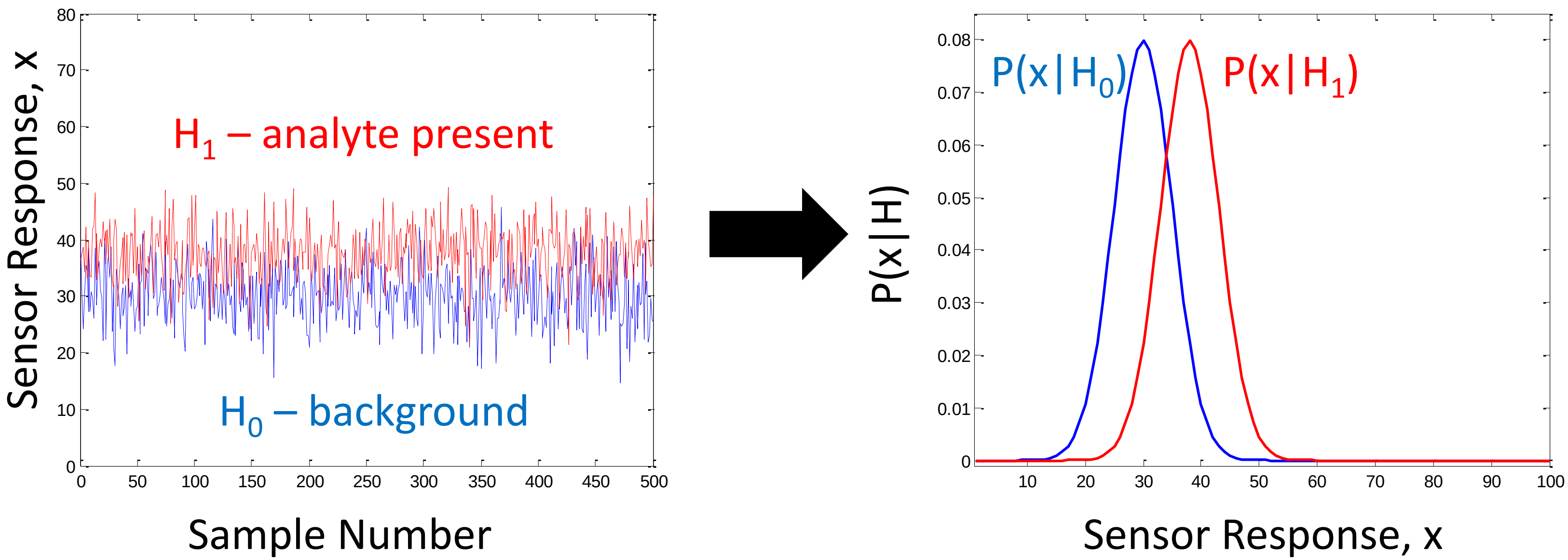
## Chemical Reactivity

Electrochemical sensors
Fluorescence Quenching
Chemical Luminescence
Colormetric sensors

# Modeling Multisensor Systems

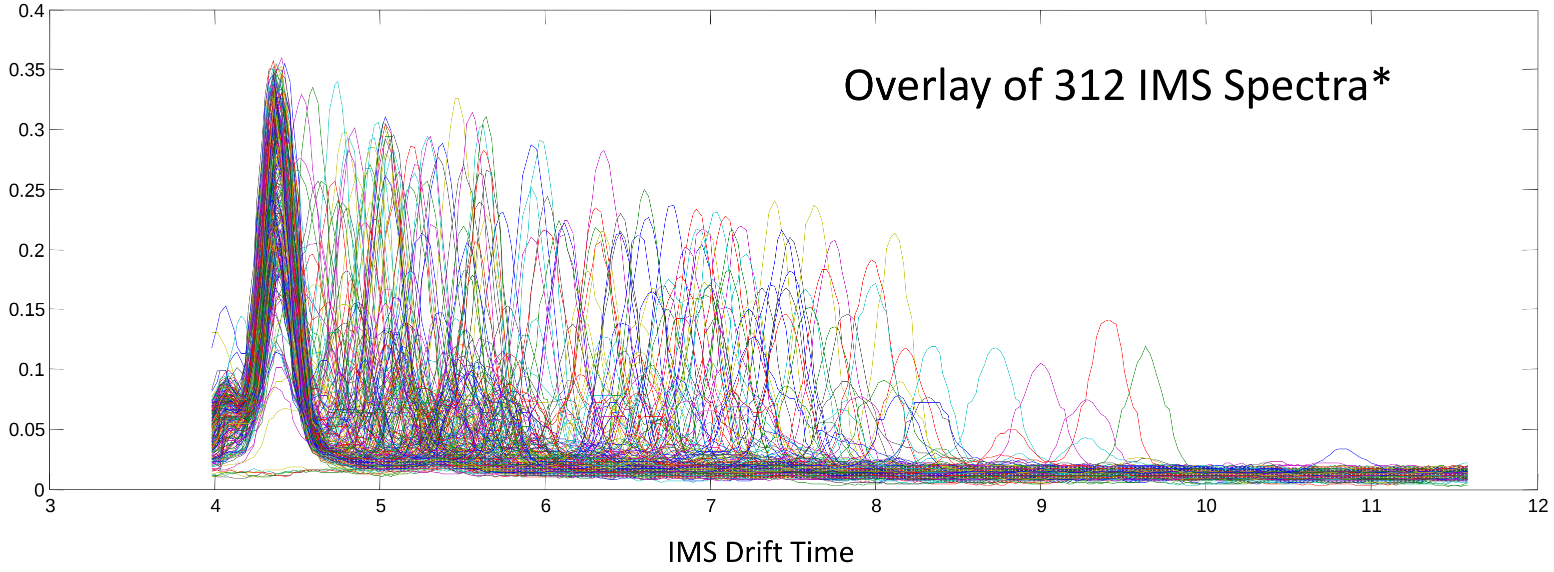
- Use known performance characteristics and library data from individual sensors
- Model sensor responses to different detection scenarios
- Combine synthetic data streams to model multisensor system response
- Test and validate multisensor system performance metric and analysis algorithms

# Univariate Sensor Data




Single channel sensors such as SAW, MEMS, etc.

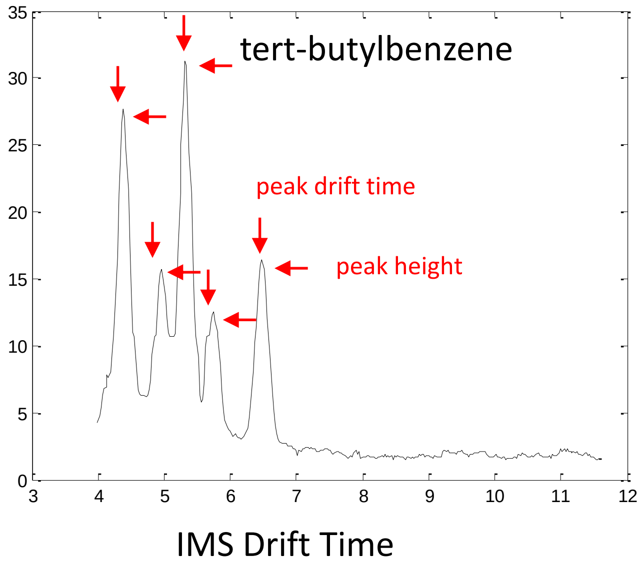
# Multivariate Sensor Data



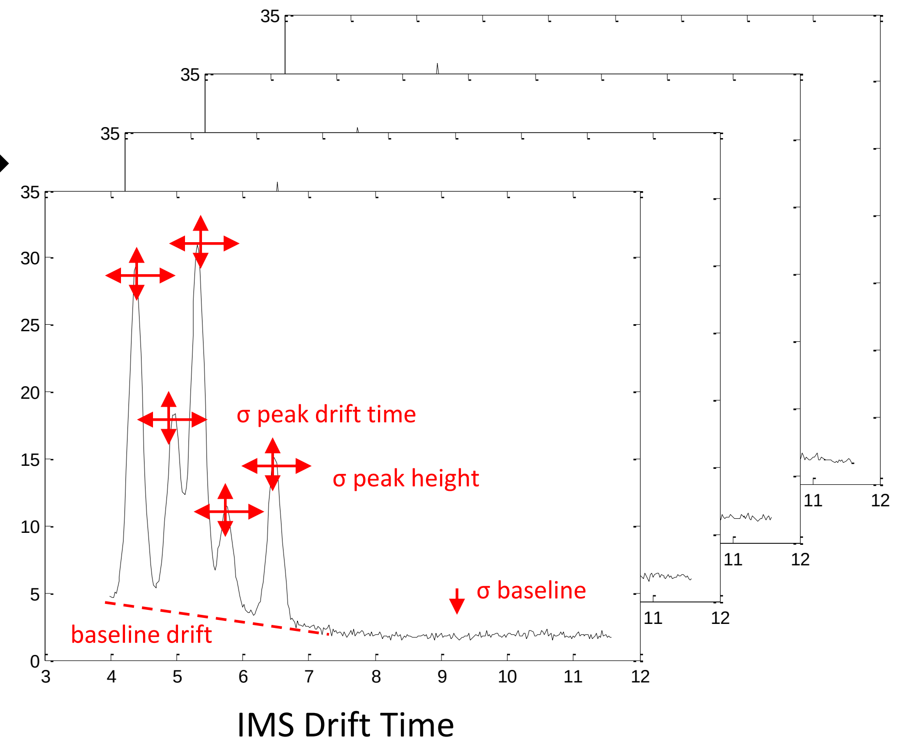

**Courtesy of Dr. Gary Eiceman at NM State University*

# Synthetic Data Generation Example

## Library IMS Data

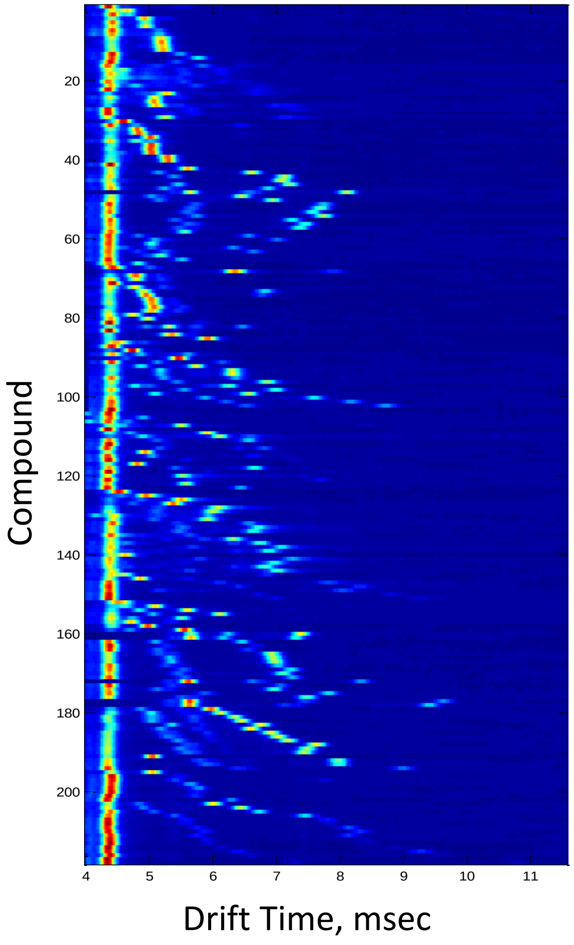



## Synthetic IMS Data

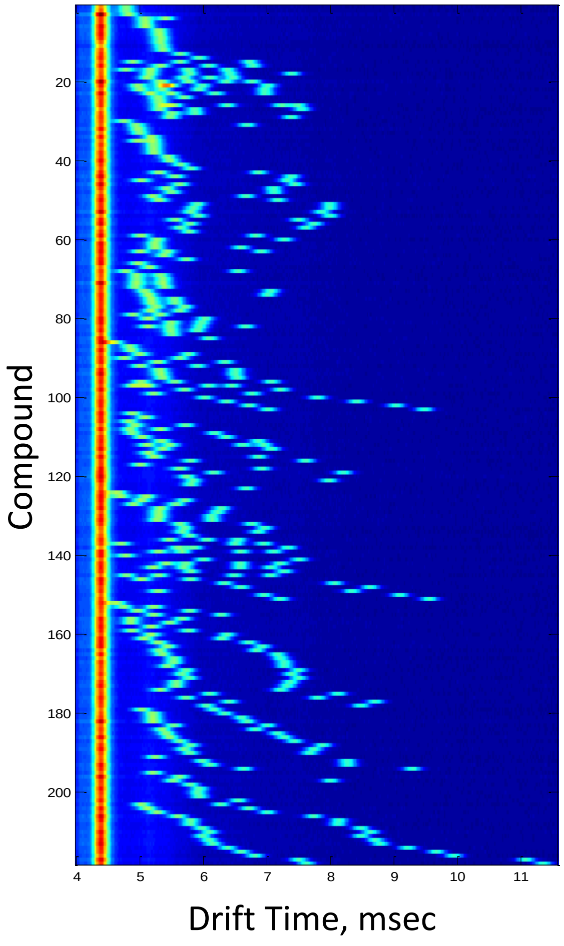


# Synthetic Data Generation Example

IMS library spectra

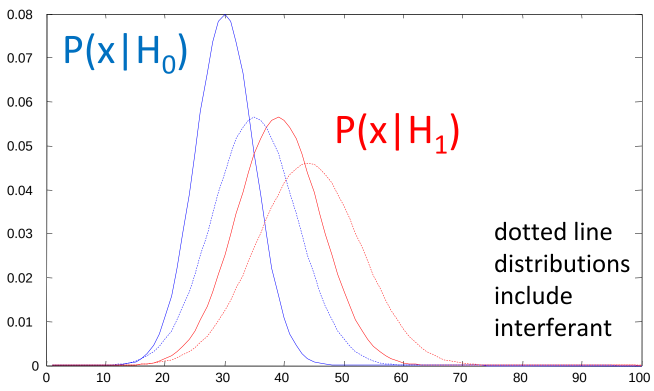



Synthetic IMS spectra

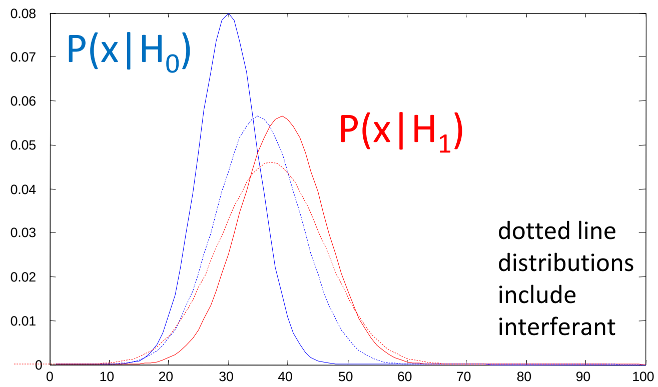


# Modes of Interference

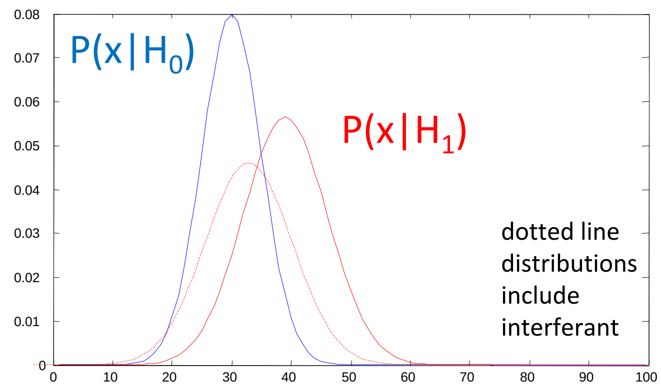
## Additive interference




## Competitive interference




## Inhibiting interference




**The presence of an interferent alters the distributions $P(x|H_0)$ and $P(x|H_1)$, and thus alters detector performance**

**The shape of the distribution of $P(x|A,I)$ will depend on the particular mode of interference**

# Example: Partially Selective Arrays

Selectivity is concentration dependant, but an array of sensors can enable improved selectivity at a range of concentrations.

There is a trade-off between detection and false alarm rates for multi-species detection in sensor arrays as individual sensor selectivity is increased or decreased.

An array of purpose-built, but still partially selective sensors can have capabilities for detecting new analytes.

More accurate estimates for real sensor parameters will improve fused system performance predictions.