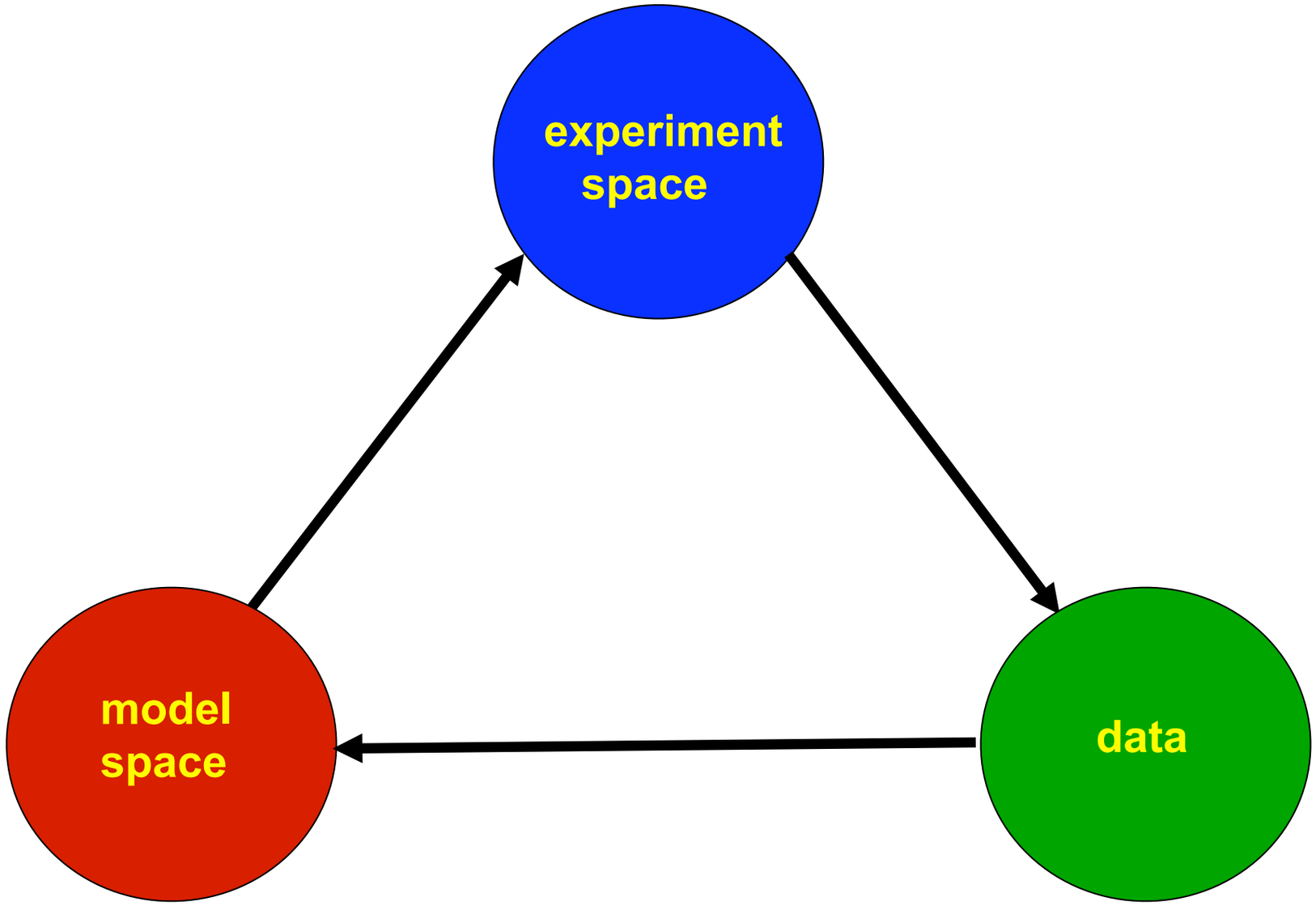
# Adaptive Information and Optimization




Rob Nowak
www.ece.wisc.edu/~nowak

WIDDOW 31 January 2011

Joint work with
R. Castro, J. Haupt, M. Malloy


WIDOW
"Echoes of White Sister, Giuffria, Icon, Surgin and Early Bon Jovi"
- Dave Ling, Classic Rock Magazine
The Critically Acclaimed Self Titled Debut Album
From Australia's Melodic Hard Rock Sensation
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# Adaptive Information

**Goal:** Estimate an unknown object $x \in \mathcal{X}$ from scalar samples

**Information**: samples of the form $y_1(x), \ldots, y_n(x)$,
the values of certain functionals of $x$

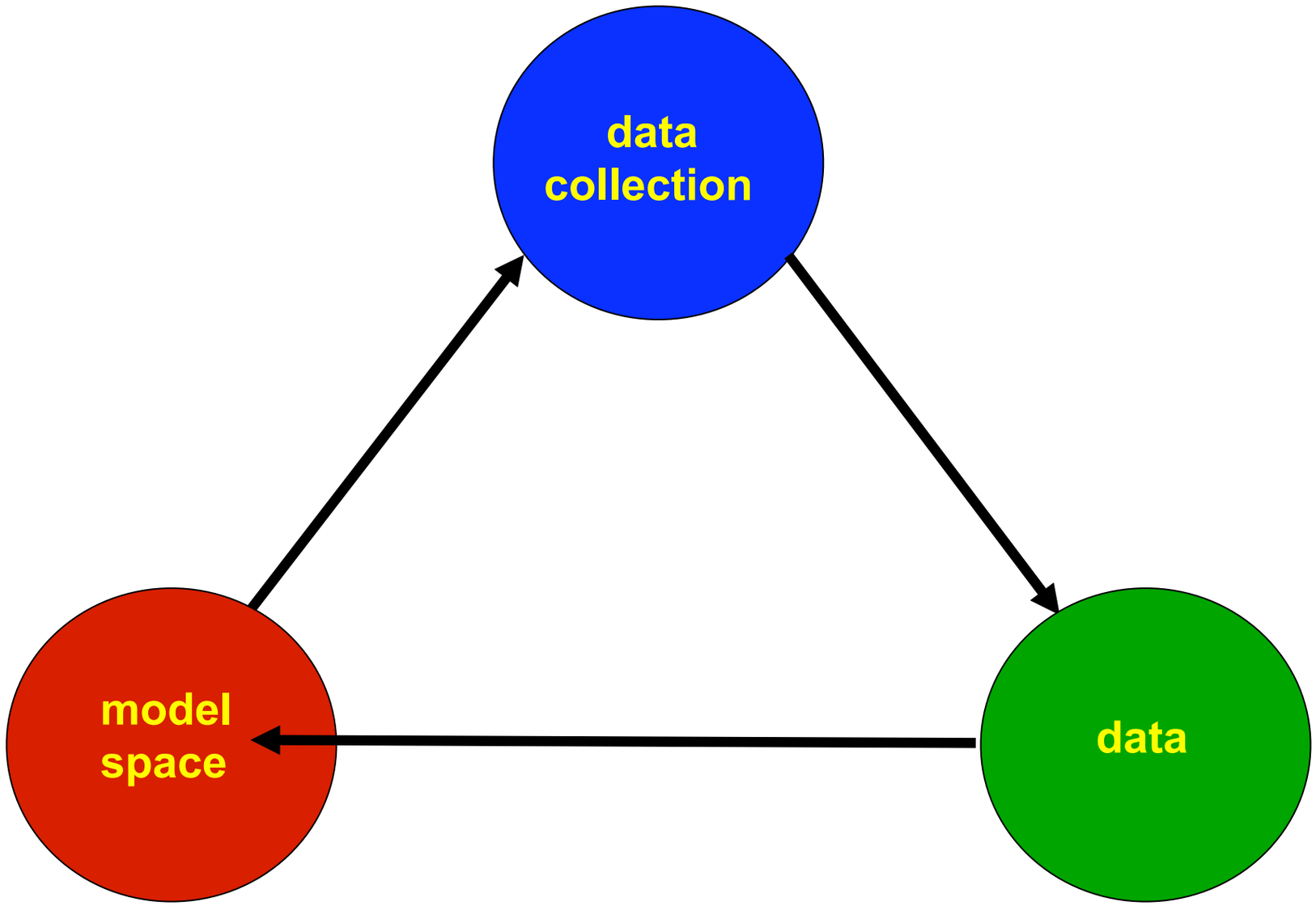
**Non-Adaptive Information**: $y_1, y_2, \cdots \in \mathcal{Y}$ non-adaptively chosen (deterministically or randomly) independent of $x$

**Adaptive Information**: $y_1, y_2, \cdots \in \mathcal{Y}$ are selected sequentially and $y_i$ can depend on previously gathered information, i.e., $y_1(x), \ldots, y_{i-1}(x)$

**Does adaptivity help?**

# Feedback from Data Analysis to Data Collection

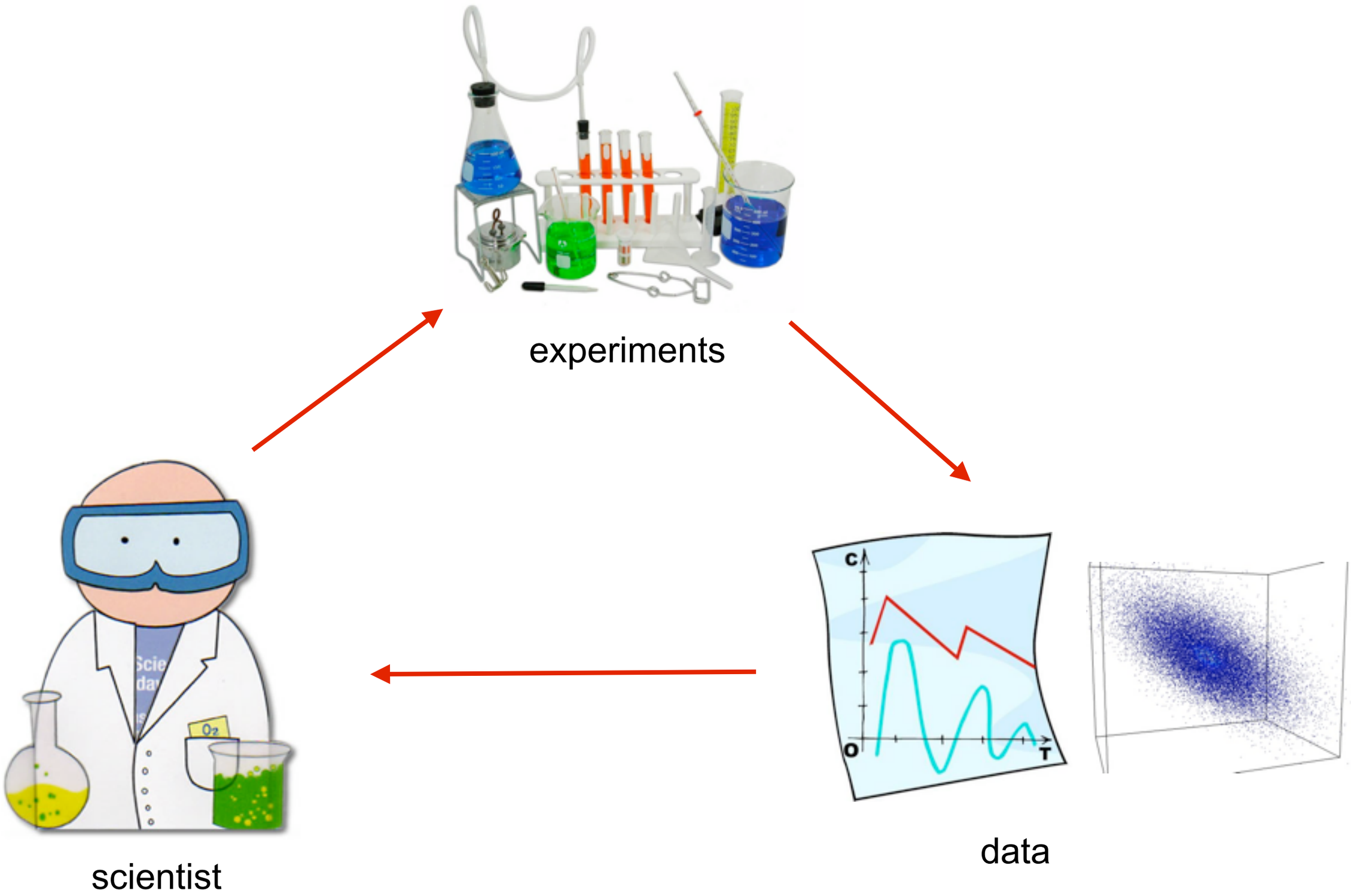
$\mathcal{Y}$: possible measurements/experiments



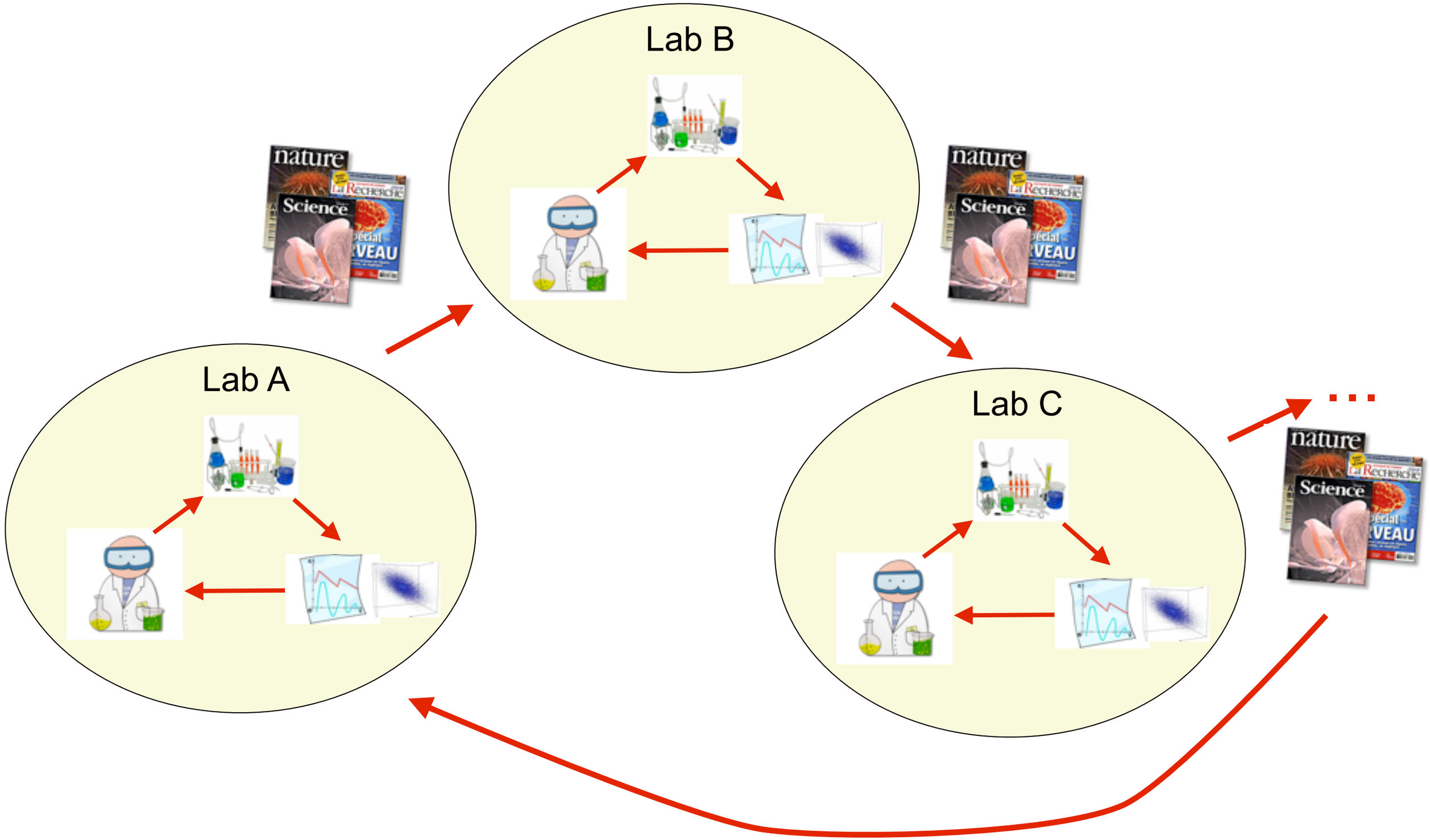

$\mathcal{X}$: models/hypotheses under consideration

$y_1(x), y_2(x), \ldots$: information/data

# The Scientific Process in a Laboratory

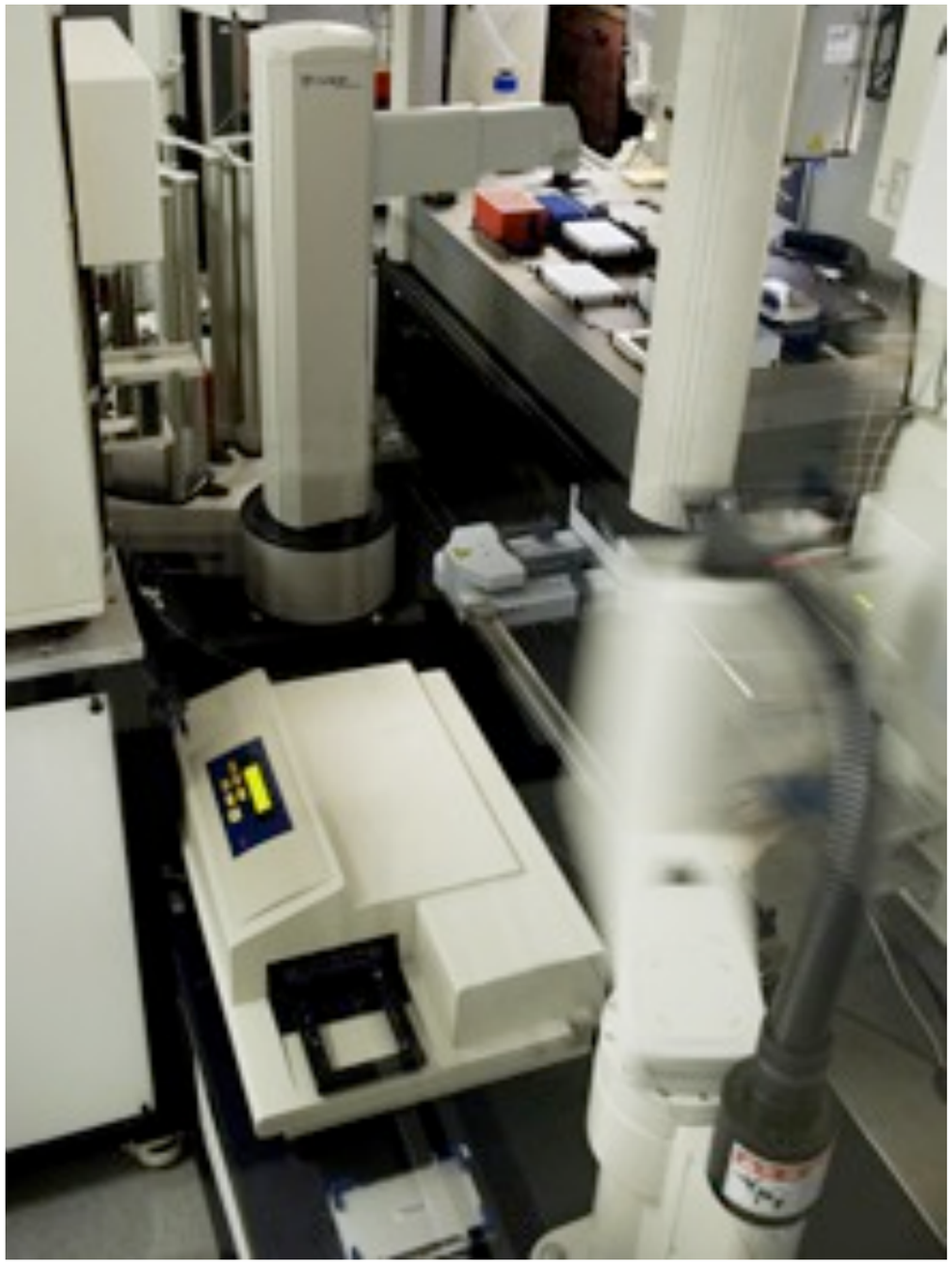


# The Scientific Process at Large



# Robot Scientist

www.aber.ac.uk/compsci/Research/bio/robotsci/



Wired Magazine, April 2009:

For the first time, a robotic system has made a novel scientific discovery with virtually no human intellectual input.

Scientists designed "Adam" to carry out the entire scientific process on its own: formulating hypotheses, designing and running experiments, analyzing data, and deciding which experiments to run next. "It's a major advance," says David Waltz of the Center for Computational Learning Systems at Columbia University. "Science is being done here in a way that incorporates artificial intelligence. It's automating a part of the scientific process that hasn't been automated in the past."

*Adam is the first automated system to complete the cycle from hypothesis, to experiment, to reformulated hypothesis without human intervention.*

# Adaptive vs. Non-Adaptive: Three Situations

The "bare minimum" number of measurements depends on intrinsic complexity of $\mathcal{X}$. In practice, the minimum number depends on jointly on $\mathcal{X}$ and $\mathcal{Y}$.

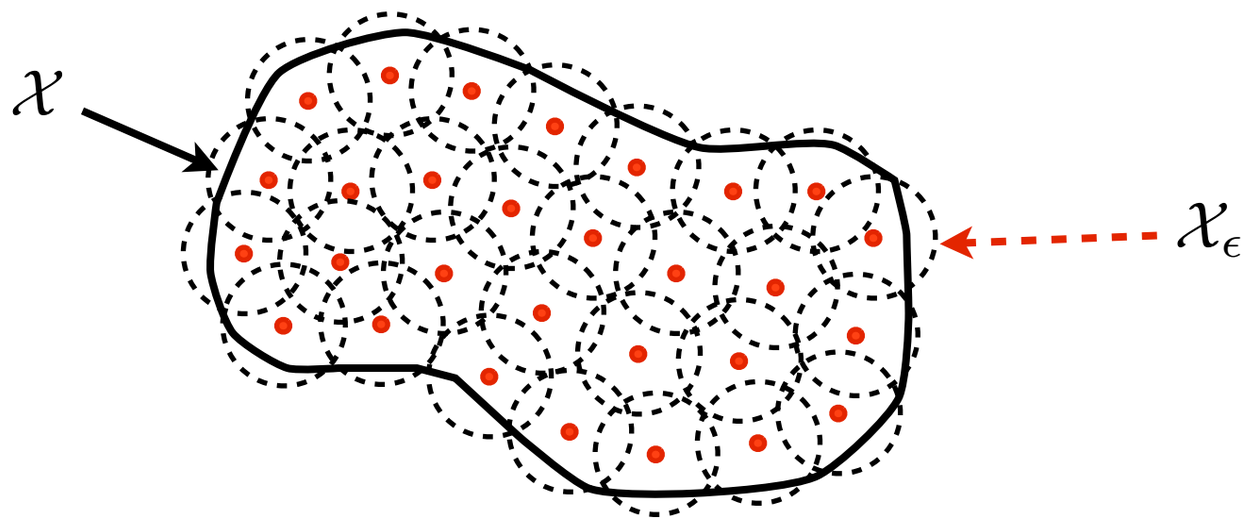
**Equal and Good**:
adaptive and non-adaptive equally informative and require about the bare minimum of measurements

**Equal and Bad**:
adaptive and non-adaptive equally (non)-informative and require many more measurements then the bare minimum

**Good and Bad**:
adaptive requires bare minimum number of measurments, non-adaptive requires many more

# The Bare Minimum

Assume $\mathcal{X}$ is equipped with metric $d$ and is compact.




Let $\mathcal{X}_\epsilon \subset \mathcal{X}$ be a finite subset of size $N_\epsilon$ having the property that any element of $\mathcal{X}$ is within distance $\epsilon$ of an element in $\mathcal{X}_\epsilon$

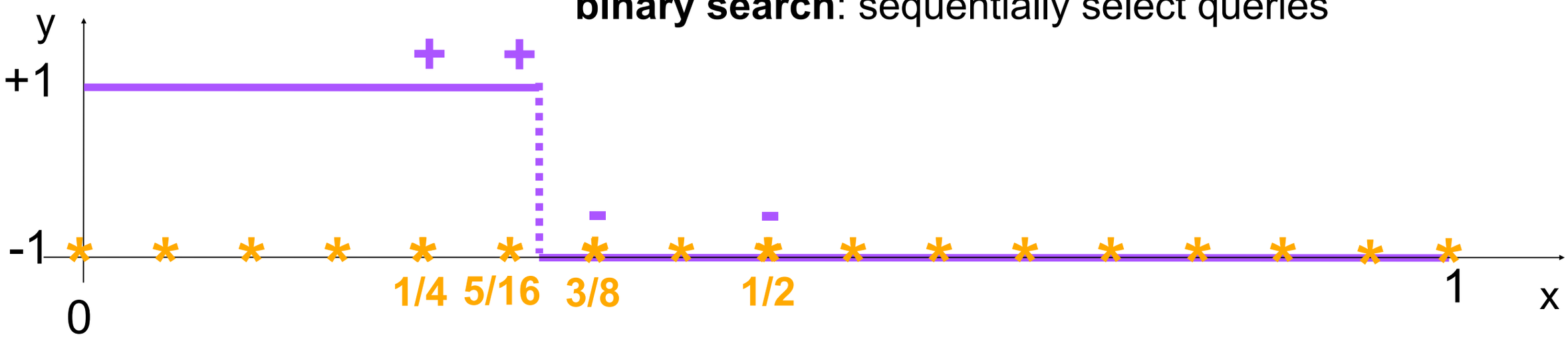
**Metric Entropy:** Need at least $\log N_\epsilon$ bits of information to approximately determine any $x \in \mathcal{X}$

Ex. suppose $\mathcal{X} = [0,1]^d$. we can take a uniform grid of points spaced $\epsilon$ apart as our cover. Then $N_\epsilon = (\frac{1}{\epsilon})^d$ and $\log N_\epsilon = d \log(1/\epsilon)$.

# Binary Search

$$\mathcal{X} = \{\text{subsets } [0, \tfrac{1}{N}], [0, \tfrac{2}{N}], \ldots, [0, 1]\}$$
$$\mathcal{Y} = \text{“membership queries”}$$

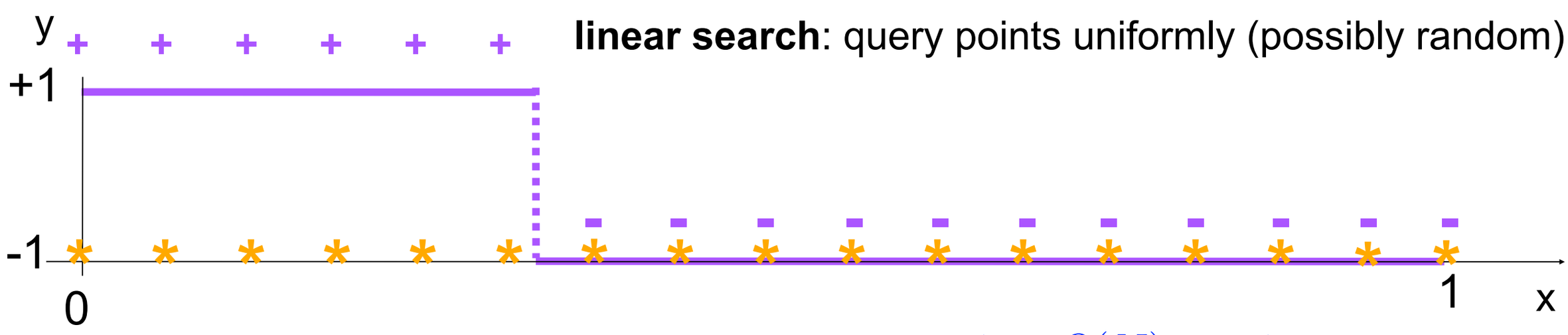
**binary search**: sequentially select queries




**1/3 = 0101…**

requires $\log_2 N$ queries

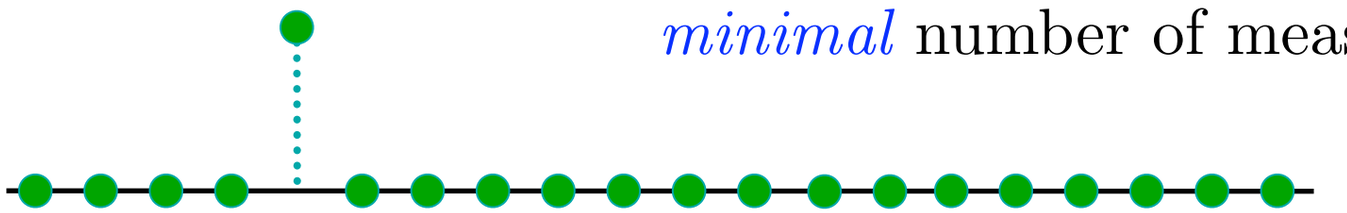
**linear search**: query points uniformly (possibly random)




requires $O(N)$ queries

# Does Adaptivity Help ?

identify a sparse signal $x \in \mathbb{R}^n$ from a *minimal* number of measurements



**Point measurments**: $y = \langle x\,,\ \delta_k \rangle = x_k$

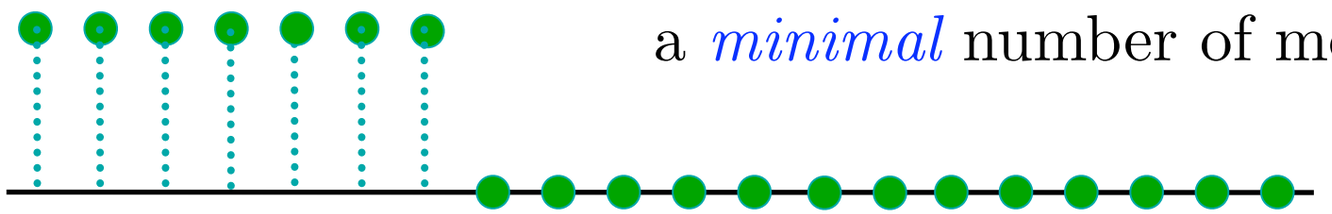
$O(n)$ measurements (random or adaptive) are needed to recover $x$

**Compressed Sensing**: $y \ = \ \langle x\,,\, \phi \rangle$ where $\phi \in \{-1, 1\}^n$

$O(\log n)$ measurements (random or adaptive) are needed to recover $x$

**Adaptivity doesn't help**

# Does Adaptivity Help ?



identify a threshold signal $x \in \mathbb{R}^n$ from a *minimal* number of measurements

**Point measurments**: $y = \langle x\,,\ \delta_k \rangle = x_k$

$O(n)$ random measurements are needed to recover $x$

$O(\log n)$ adaptive measurements are needed to recover $x$ (binary search)

**Compressed Sensing**: $y \ = \ \langle x\,,\, \phi \rangle$ where $\phi \in \{-1, 1\}^n$

$O(\log n)$ random measurements are needed to recover $x$

**Adaptivity may help, depending on nature of signal and measurements**

# Optimizing Information Collection

**Goal:** Estimate an unknown object $x \in \mathcal{X}$ from scalar samples

**Information**: samples of the form $y_1(x), \ldots, y_n(x)$,
the values of certain functionals of $x$

**Adaptive Information**: $y_1, y_2, \cdots \in \mathcal{Y}$ are selected sequentially and $y_i$ can depend on previously gathered information, i.e., $y_1(x), \ldots, y_{i-1}(x)$

**Dynamic Programming:** $K > 0$ measurement/experiment steps

$$\min_{\widehat{x}\,,\, y_1,\ldots,y_K} \; \max_{x \in \mathcal{X}} \; d(x\,,\, \widehat{x}(y_1, \ldots, y_K))$$

computationally prohibitive in all but very low-dimensional, simple problems

# Greedy Strategies

**Ex. Binary Information:** for each $x \in \mathcal{X}$ and $y \in \mathcal{Y}$,

$$y(x) = \begin{cases} +1 & , \quad \text{if } x \text{ predicts a positive outcome on } y \\ -1 & , \quad \text{if } x \text{ predicts a negative outcome on } y \end{cases}$$

optimal procedure is a search tree; construction is NP-complete (Hyafil & Rivest '76)

**Splitting Algorithm**

initialize: $n = 0$, $\mathcal{X}_0 = \mathcal{X}$

while $|\mathcal{X}_n| > 1$

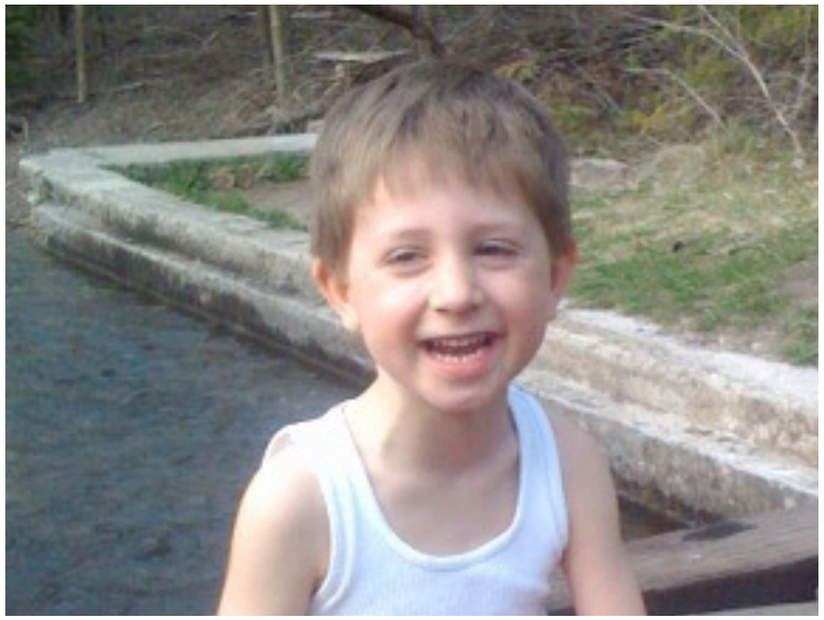
1) Select $y_n = \arg\min_{y \in \mathcal{Y}} |\sum_{x \in \mathcal{X}_n} y(x)|$

2) Perform $y_n$ to obtain information $y_n(x^*)$

3) Set $\mathcal{X}_{n+1} = \{x \in \mathcal{X}_n : y_n(x) = y_n(x^*)\}$, $n = n + 1$

Splitting Algorithm is near-optimal (average depth is within $\log |\mathcal{X}|$ factor of optimal)

**depth of optimal tree depends on nature of $\mathcal{X}$ and $\mathcal{Y}$**

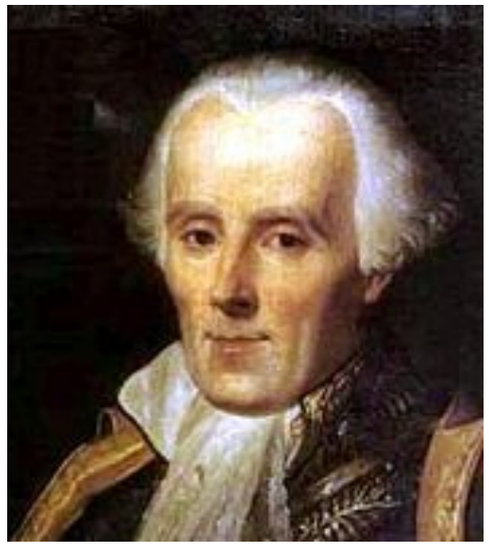



“Is the person wearing a hat ?”

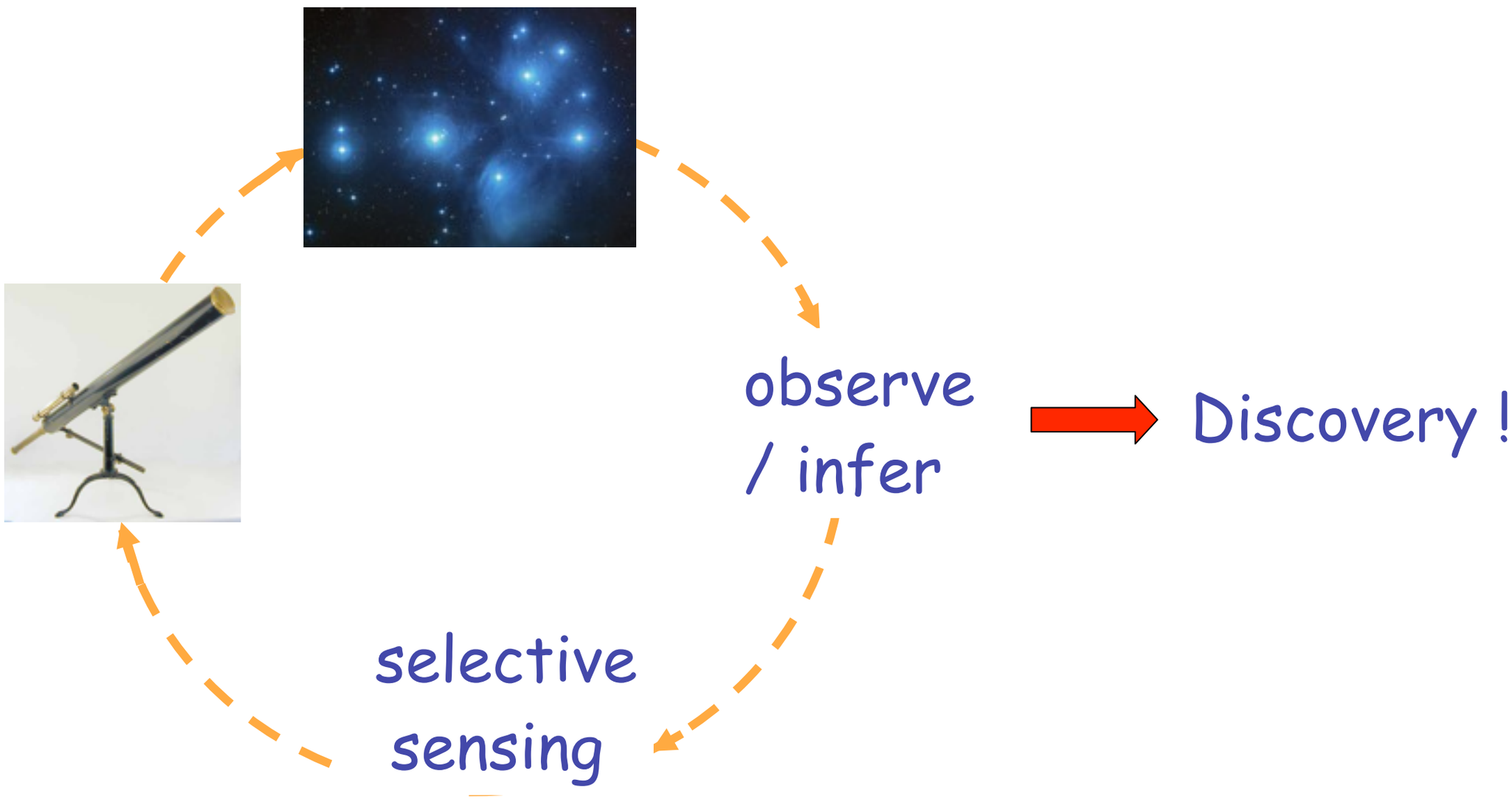
“Does the person have blue eyes ?”

splitting algorithm is quite effective if responses are reliable

# Laplace



Decided to make new astronomical measurements when “the discrepancy between prediction and observation [was] large enough to give a high probability that there is something new to be found.”  Jaynes (1986)



# Probabilistic Splitting Algorithm

**Probabilistic Splitting Algorithm**

initialize: $p_0(x) =$ uniform

for $n = 0, 1, \ldots, k-1$

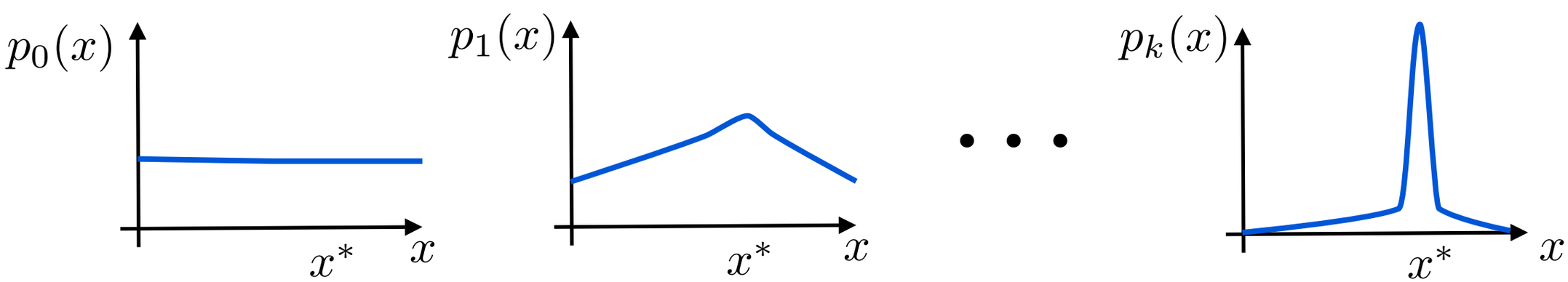
1) Select $y_{n+1}$ to maximize $\mathbb{E}_y \left[ \int p_n(x|y) \log \frac{p_n(x|y)}{p_n(x)} \, dx \right]$

2) Perform $y_{n+1}$ to obtain information $y_{n+1}(x^*)$

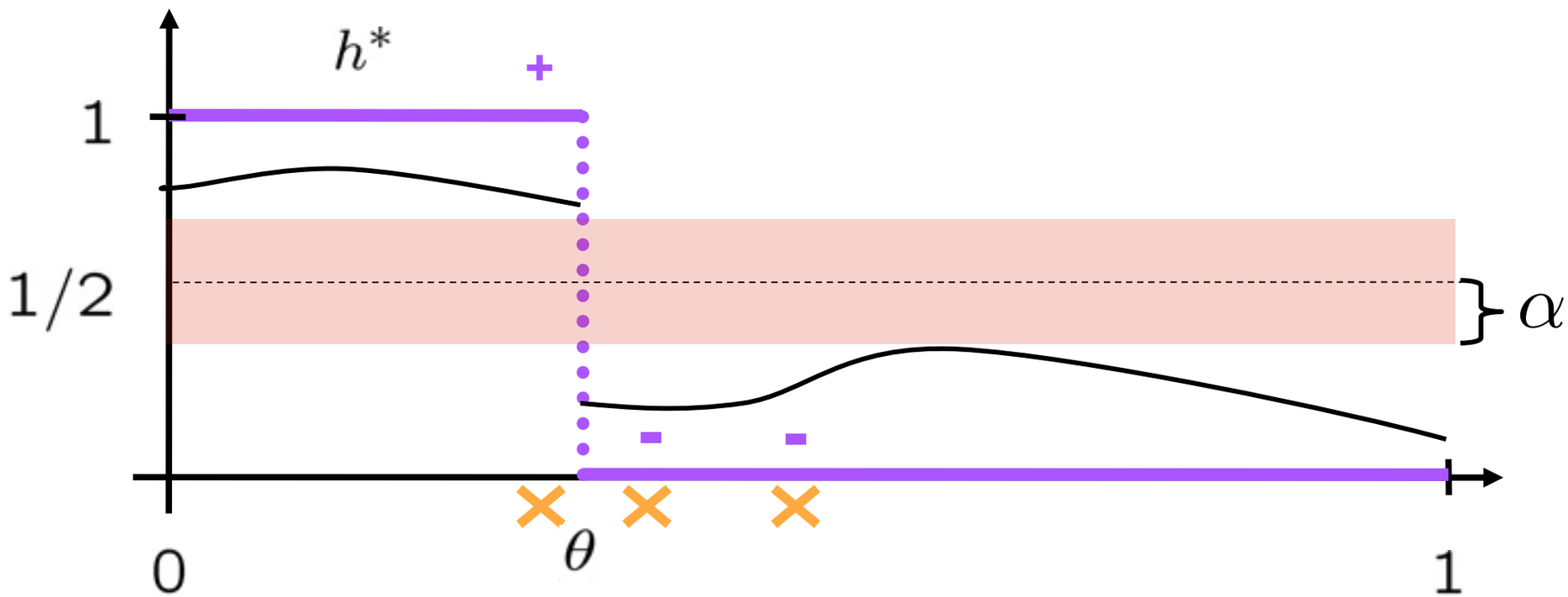
3) $y_{n+1}(x^*)$ + Bayes rule: $p_n(x) \to p_{n+1}(x)$

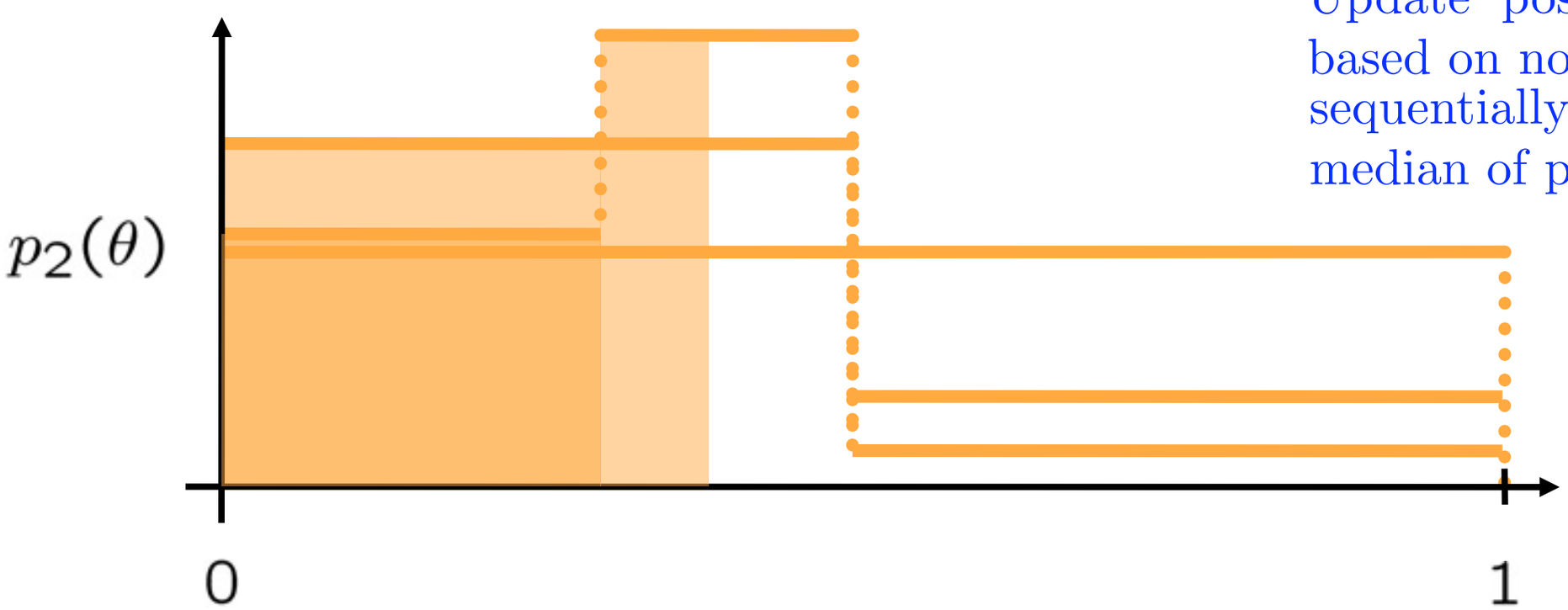
output: $\arg\max_x p_k(k)$

**"Information-Gain"**
(Shannon '48, Lindley '56)



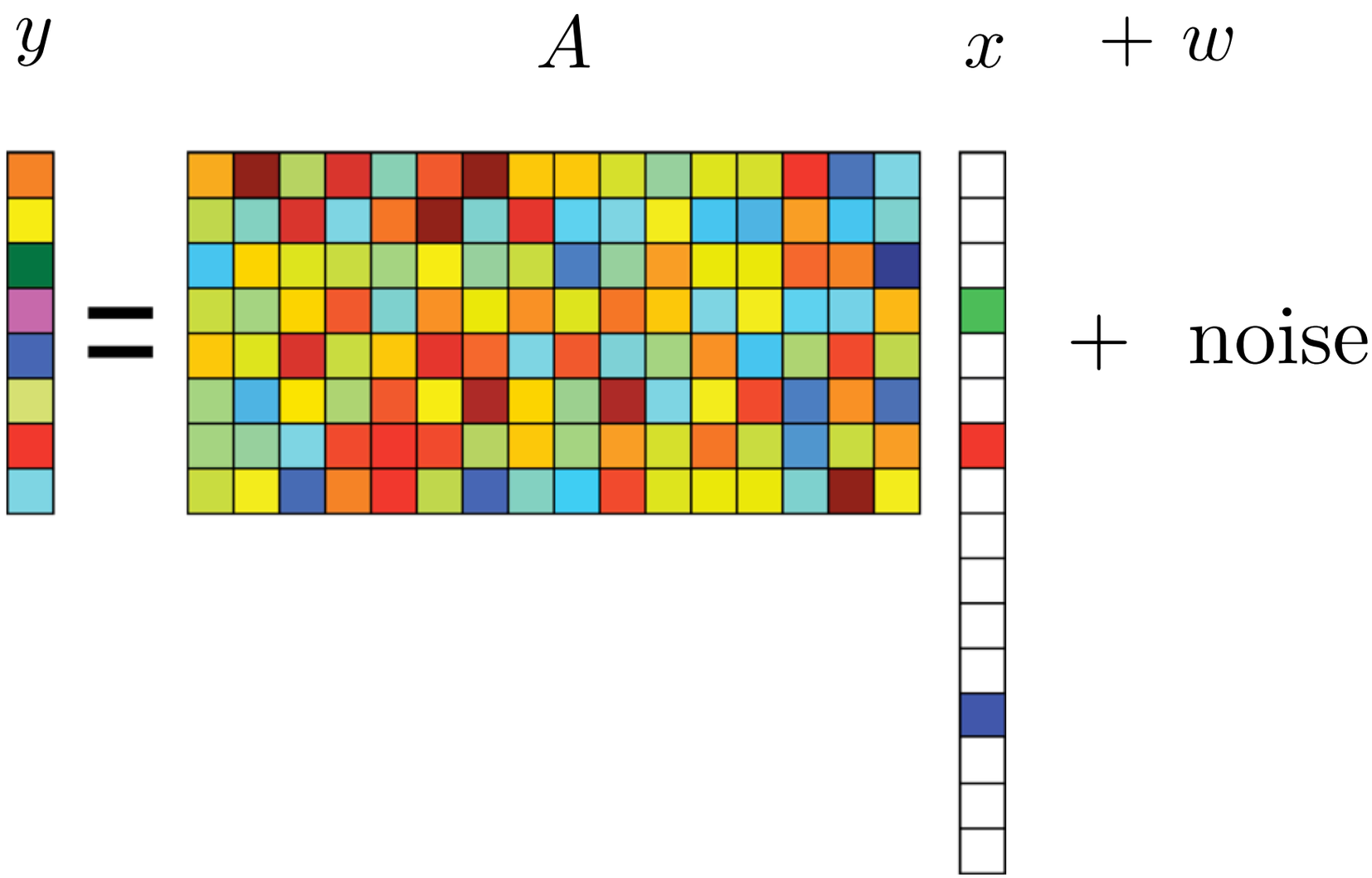
# Ex. Noisy Binary Search (Burnashev & Zigangirov '74)




Update 'posterior' density based on noise bound $\alpha$ sequentially take samples at median of posterior density

# Sparsity and High-Dimensional Models




$y \;=\; A\,x \;+\; w$ , with $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$ (but sparse), $w \sim \mathcal{N}(0, I)$

# Signal Processing Gear

back to shop

## y = phi x (Dark T-Shirt)

$18.99

**Fit:** Standard

Not too tight, not too loose.

**Fabric Thickness:**

Thin — Thick

1. Color: (Charcoal)
2. Size: Large — Size Chart
3. Qty: 1

**ADD TO CART**

AVAILABILITY: In Stock.
Product Number: 030-469487567

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A visual representation of the math behind compressive sensing

Look cool without breaking the bank. Our durable, high-quality, pre-shrunk 100% cotton t-shirt is what to wear when you want to go comfortably casual. Preshrunk, durable and guaranteed.

- 5.6 oz. 100% cotton
- Standard fit

### Other items by Signal Processing Gear:

y = phi x (Mug)

y = phi x (Large Mug)

y = phi x (Light T-Shirt)

# Experimental Design

$$y \;=\; Ax \;+\; w$$

experimental design: how to design $A$ ?

**Constraints:**

- sample budget: $A$ is $m \times n$ with $m \leq k < n$
- precision budget: $\|A\|_F^2 \leq$ Constant

**Sequential Design:** how to chose $A_1, \ldots, A_k$ to max prob of identifying $x$?

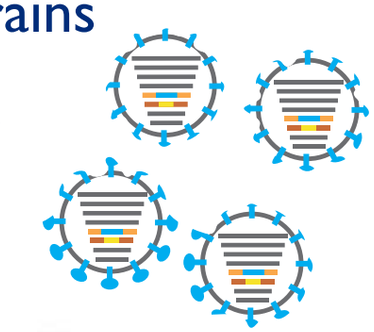
$$\begin{aligned} y_1 &= A_1 x + w_1 \\ y_2 &= A_2 x + w_2 \\ &\vdots \\ y_k &= A_k x + w_k \end{aligned}$$

# Application: Inferring Biological Pathways

virus

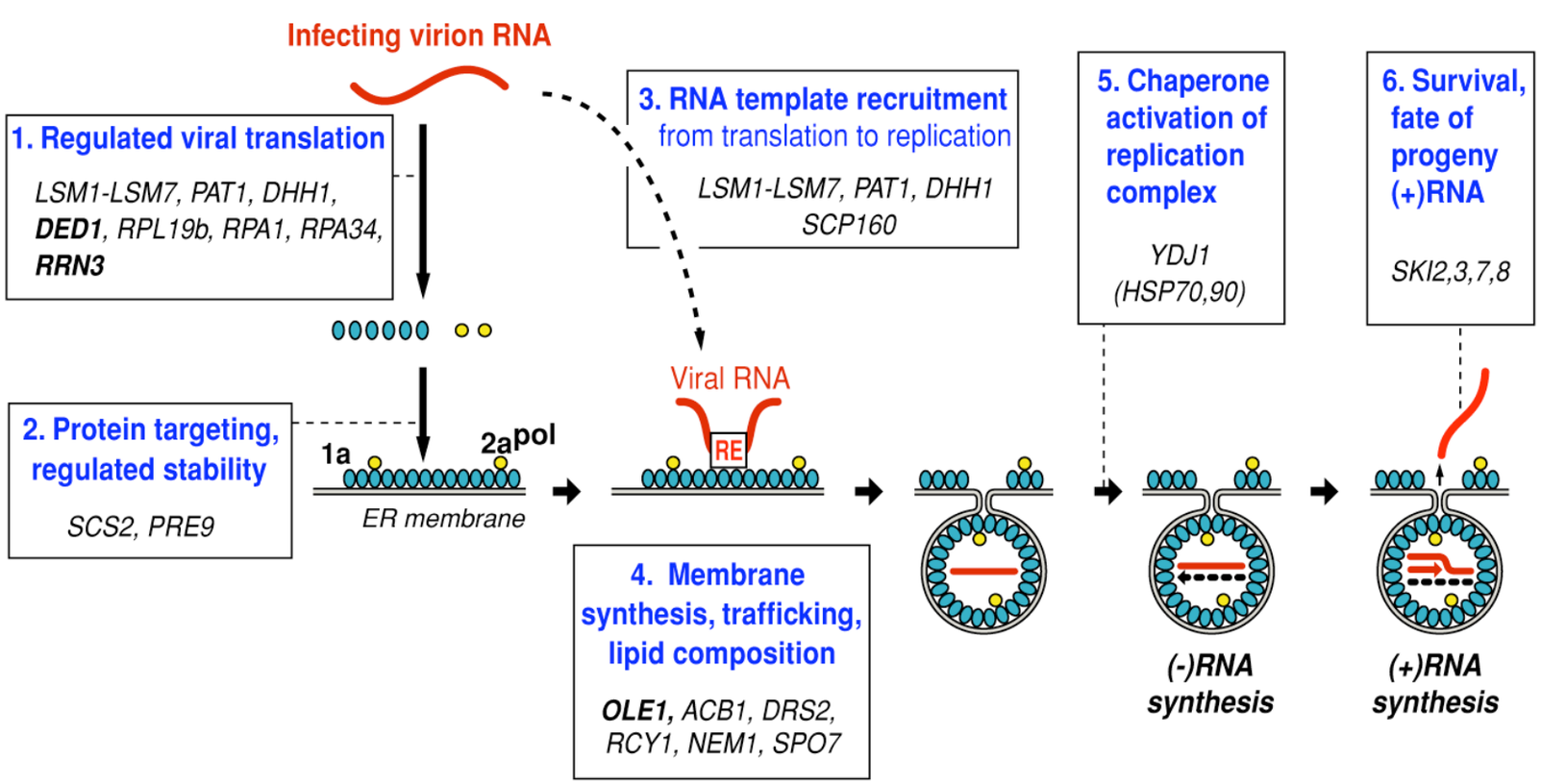
fruit fly

13,071 single-gene knock-down cell strains



infect each strain with fluorescing virus

microwell array




approximately 100 significant genes/protiens discovered by Ahlquist and Kawaoka Labs at UW-Madison

# Challenge: High-Dimensionality and Low SNR

nature Vol 454|14 August 2008|doi:10.1038/nature07151

## *Drosophila* RNAi screen identifies host genes important for influenza virus replication

Linhui Hao[1,2]*, Akira Sakurai[3]*†, Tokiko Watanabe[3], Ericka Sorensen[1], Chairul A. Nidom[5,6], Michael A. Newton[4], Paul Ahlquist[1,2] & Yoshihiro Kawaoka[3,7,8,9]

How do they confidently determine the ~100 out of 13K genes hijacked for virus replication from extremely noisy data?

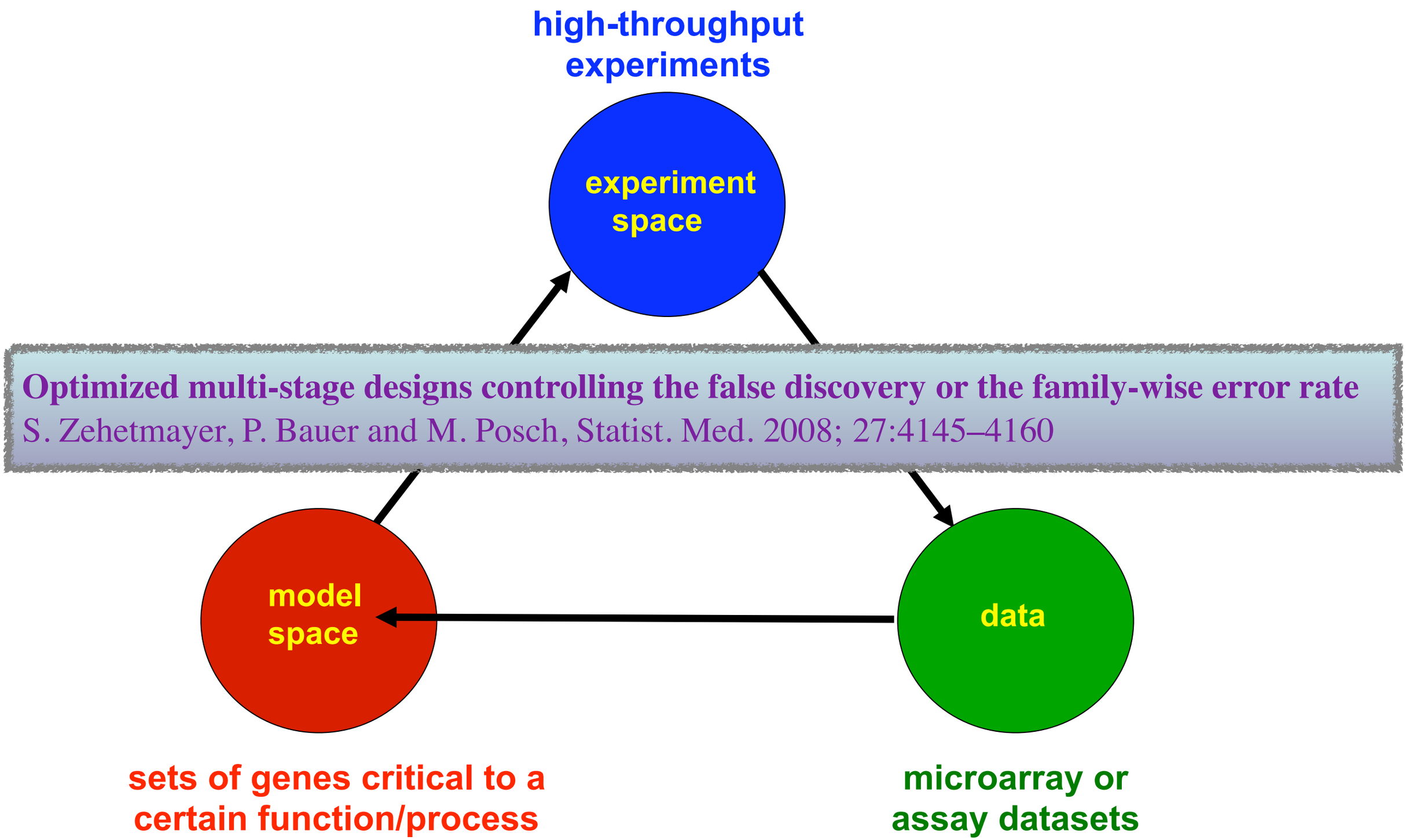
**Sequential Experimental Design:**

**Stage 1**: assay all 13K strains, twice; keep all with significant fluorescence in one or both assays for 2nd stage (13K $\rightarrow$ 1K)

**Stage 2**: assay remaining 1K strains, 6-12 times; retain only those with statistically significant fluorescence (1K $\rightarrow$ 100)

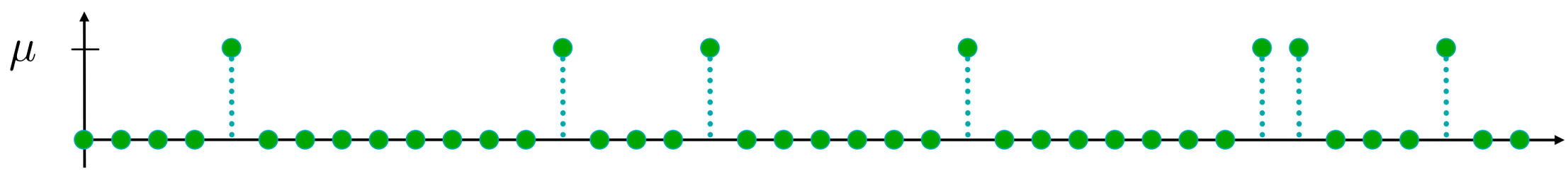
vastly more efficient that replicating all 13K experiments many times

# Feedback from Data Analysis to Data Collection



# Sparse Signal Model

Let $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$ be an unknown sparse vector;
most (or all) of its components $x_i$ are equal to zero.




$$x_i = \begin{cases} \mu > 0\,, & i \in \mathcal{S} \\ 0\,, & i \notin \mathcal{S} \end{cases}, \text{ where } |\mathcal{S}| \ll n$$

signal **support set**

deterministic
but unknown

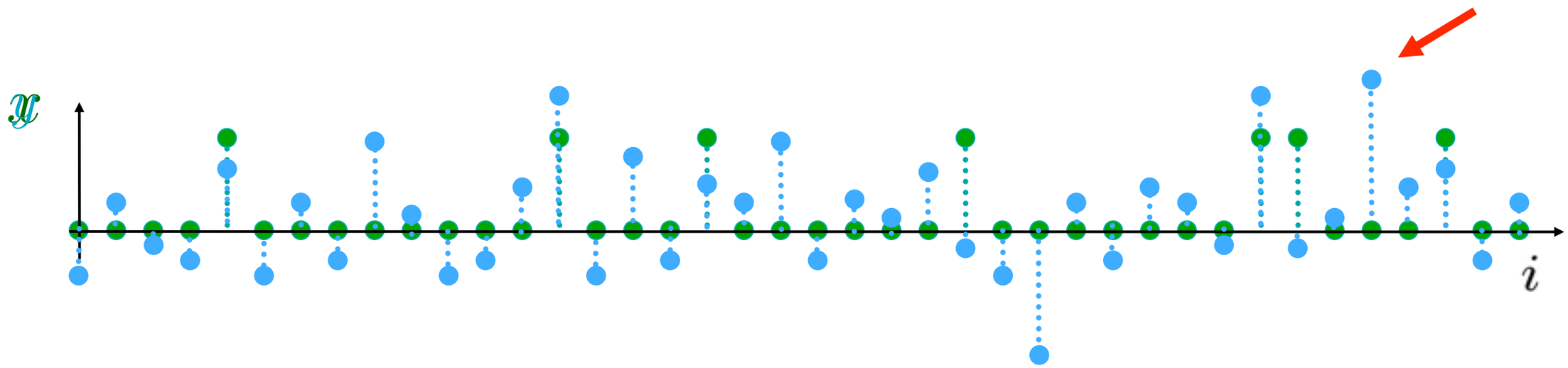
**Assume sublinear sparsity level:** $|\mathcal{S}| \ll n$

number of signal
components

# Noisy Observation Model

$$y_i \;=\; x_i \;+\; z_i\,,\;\; i = 1, \ldots, n$$

$$z_i \;\overset{\text{iid}}{\sim}\; \mathcal{N}(0,1)$$



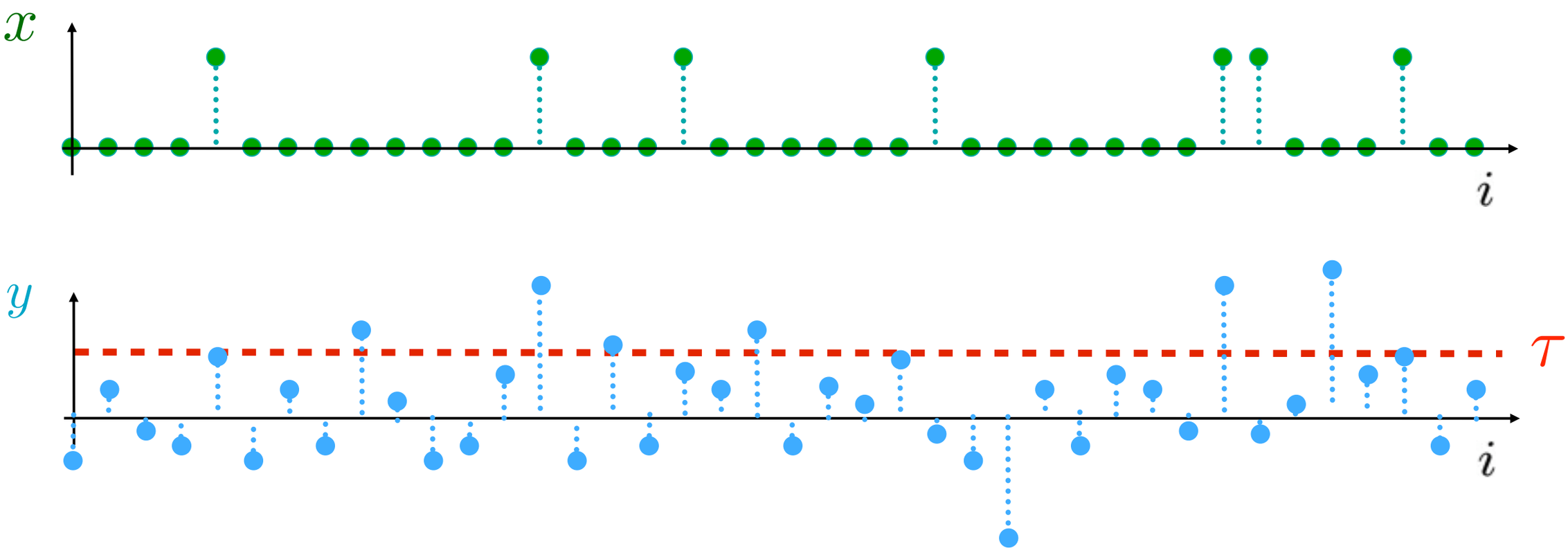

Suppose we want to locate just **one** signal component: $\widehat{i} \;=\; \arg\max_i y_i$

Even if no signal is present, $\max_i y_i \;\sim\; \sqrt{2\log n}$

**It is *impossible* to reliably detect signal components weaker than $O(\sqrt{\log n})$**

# Threshold Tests

Our goal is to estimate the set of non-zero components: $\mathcal{S} := \{i \,:\, x_i \neq 0\}$




**Definition 1** *A* threshold test *is an estimator of the form:*

$$\widehat{\mathcal{S}}_\tau(y) \;:=\; \{i \in \{1, \ldots, n\} : y_i \geq \tau > 0\}$$

**Bonferroni Correction**: To keep the error level small (e.g., less than 5%) the threshold must be on the order of $\sqrt{\log n}$.

# Is there really a problem ?

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News for Your Neurons
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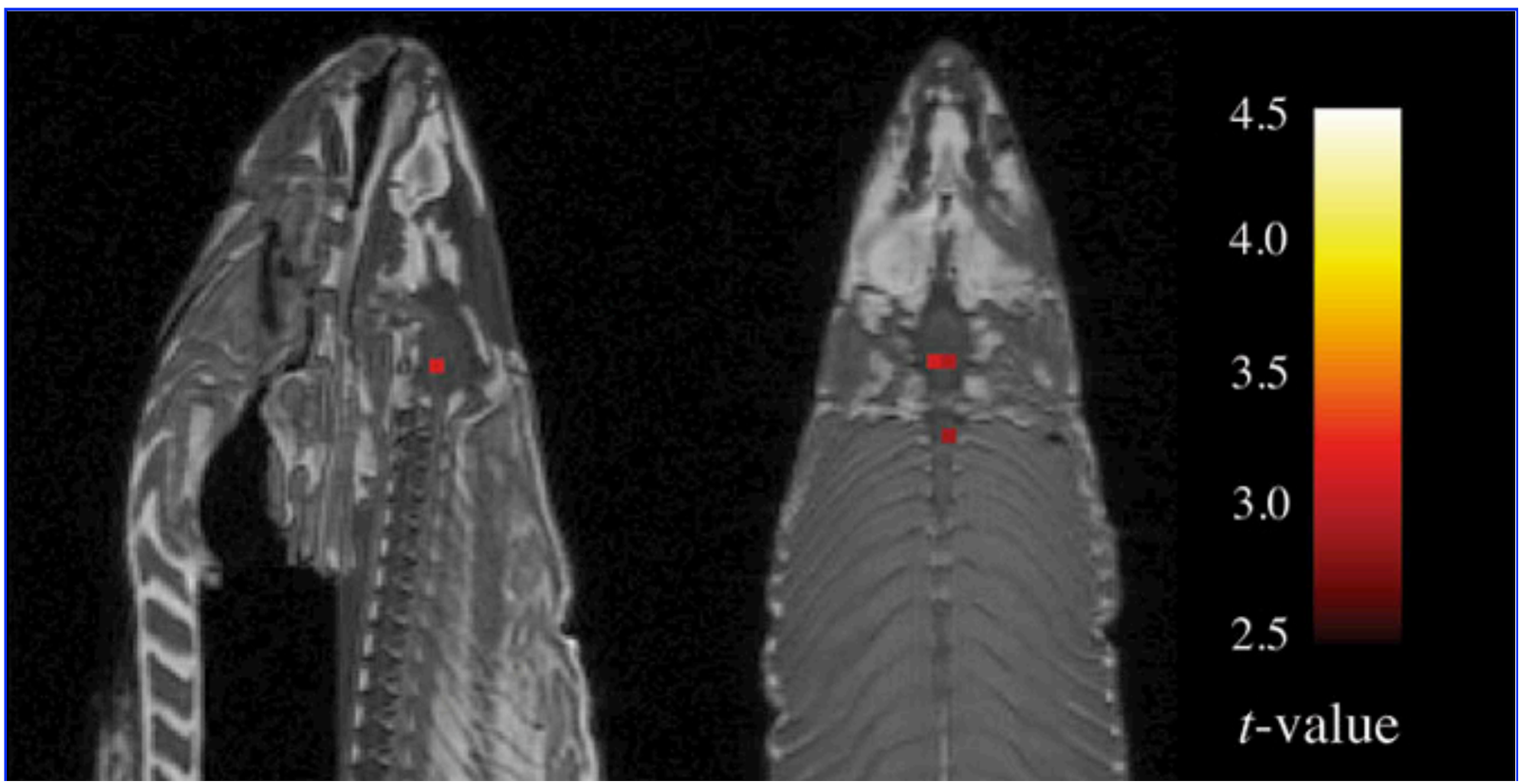
## Scanning Dead Salmon in fMRI Machine Highlights Risk of Red Herrings

By Alexis Madrigal September 18, 2009 | 5:37 pm | Categories: Brains and Behavior



# An Alternative: Sequential Experimental Design

Instead of the usual non-adaptive observation model

$$y_i \;=\; x_i \;+\; z_i\,,\;\; i = 1, \ldots, n$$

suppose we are able to sequentially collect several independent measurements of each component of $x$, according to

$$y_{i,j} \;=\; x_i \;+\; \gamma_{i,j}^{-1/2}\, z_{i,j}, \quad i = 1, \ldots, n, \;\; j = 1, \ldots, k$$

where

$j$ indexes the measurement steps

$k$ denotes the total number of steps

$z_{i,j} \overset{\text{iid}}{\sim} \mathcal{N}(0, 1)$

$\gamma_{i,j} \geq 0$ controls the precision of each measurement

**Total precision budget is constrained, but the choice of $\gamma_{i,j}$ can depend on past observations $\{y_{i,\ell}\}_{\ell<j}$.**

# Experimental (Precision) Budget

sequential measurement model

$$y_{i,j} \;=\; x_i \;+\; \gamma_{i,j}^{-1/2}\, z_{i,j}, \quad i = 1, \ldots, n, \quad j = 1, \ldots, k$$

The precision parameters $\{\gamma_{i,j}\}$ are required to satisfy

$$\sum_{j=1}^{k} \sum_{i=1}^{n} \gamma_{i,j} \;\leq\; n$$

For example, the usual non-adaptive, single measurement model corresponds to taking $k = 1$, and $\gamma_{i,1} = 1$, $i = 1, \ldots, n$. This baseline can be compared with adaptive procedures by allowing $k > 1$ and variable $\{\gamma_{i,j}\}$ satisfying budget.

**Precision parameters control the SNR per component.**

SNR is increased/decreased by

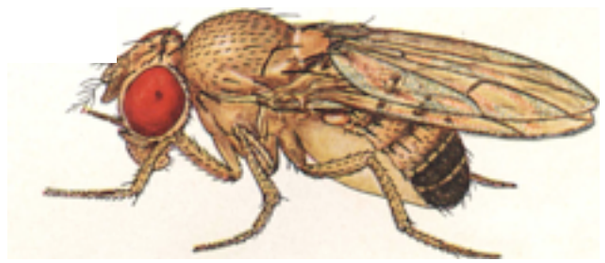
— more/fewer repeated samples or

— longer/shorter observation times

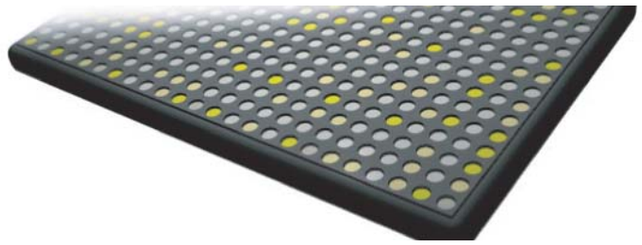
# Fruit Fly Example

virus

fruit fly



assay



How to find genes involved in virus replication ?

**Sequential Design Idea**

Budget: **k assays**, n tests/assay

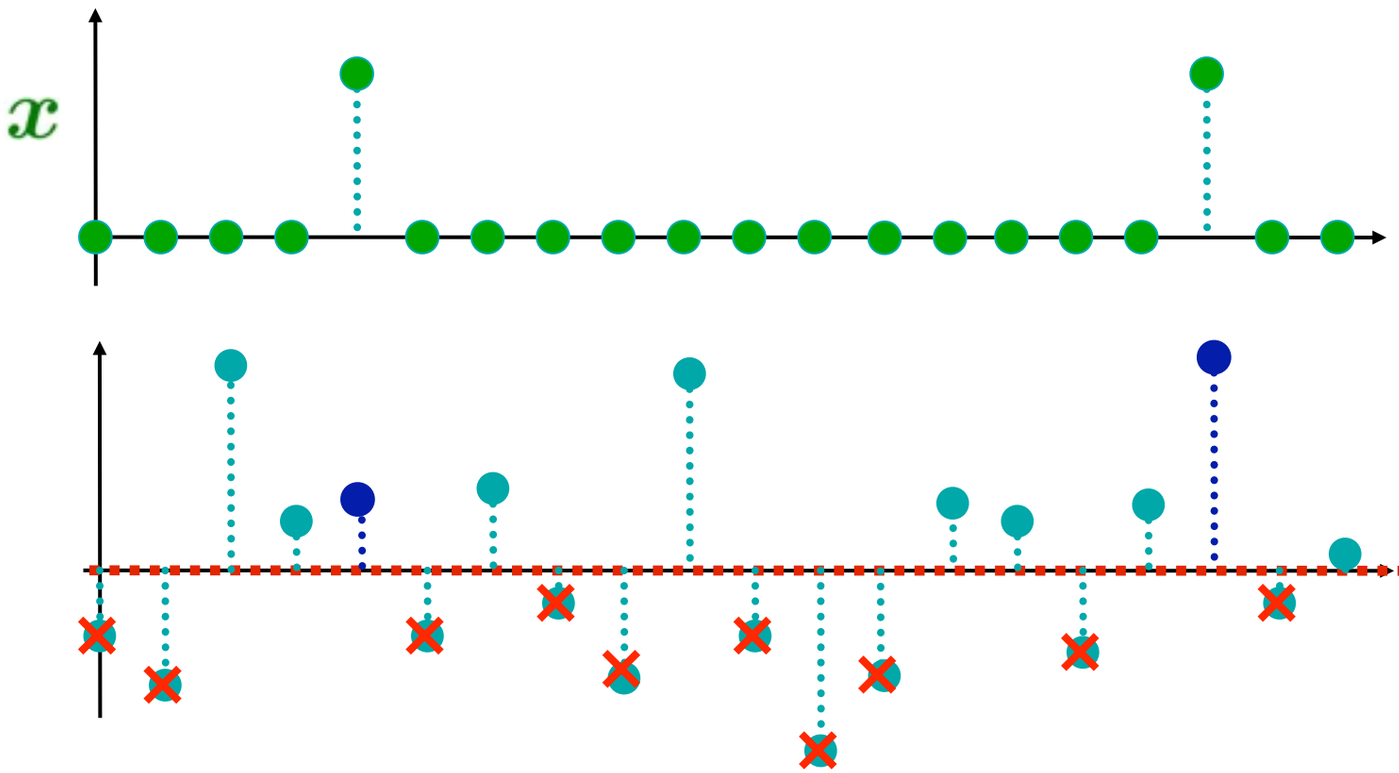
**Assay 1**: measure fluorescence of all n genes; discard n/2 genes with weakest fluorescence.

**Assay 2**: measure fluorescence for remaining n/2 genes, each tested twice (double SNR); discard n/4 genes with weakest fluorescence.

**Assay 3**: measure fluorescence for remaining n/4 genes, each tested four times (quadruple SNR); discard n/8 genes with weakest fluorescence.

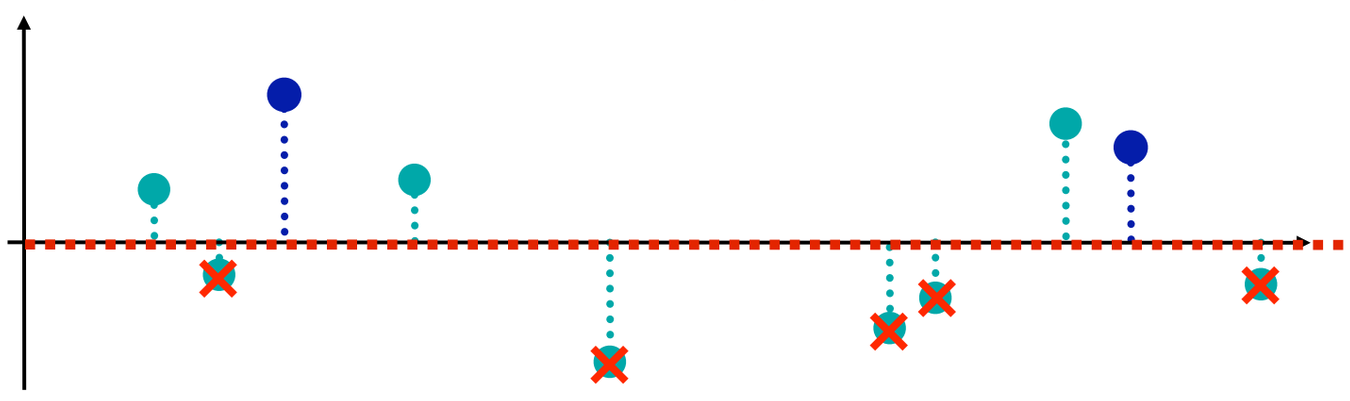
continue "distilling"....

# Idealized Example




Take $k = 3$ steps and split precision budget uniformly ($n/3$ per step)

$$y_{i,1} = x_i + \mathcal{N}(0, 3)$$



$$y_{i,2} = x_i + \mathcal{N}\left(0, \frac{3}{2}\right)$$

$$y_{i,3} = x_i + \mathcal{N}\left(0, \frac{3}{4}\right)$$

# Distilled Sensing

***Simple* Distilled Sensing**

initialize: $\mathcal{S}_0 = \{1, \ldots, n\}$, $\gamma_{i,j}^{-1} = 2 + \epsilon$, $\epsilon > 0$

for $j = 1, \ldots, k$

1) measure: $y_{i,j} \sim \mathcal{N}(x_i, 2 + \epsilon)$ , $i \in \mathcal{S}_{j-1}$

2) threshold: $\mathcal{S}_j = \{i : y_{i,j} \geq 0\}$

end

output: $\mathcal{S}_k = \{i : y_{i,k} > 0\}$

total precision budget: $\mathbb{E}\left[\sum_{i,j} \gamma_{i,j}\right]$

$$
\begin{aligned}
&= \frac{1}{2+\epsilon} \sum_{j=1}^{k} \mathbb{E}|\mathcal{S}_{j-1}| \\
&\leq \frac{1}{2+\epsilon} \sum_{j=1}^{k} \left( \frac{n - |\mathcal{S}|}{2^{j-1}} + |\mathcal{S}| \right) \\
&\leq \frac{2(n - |\mathcal{S}|)}{2+\epsilon} + k|\mathcal{S}| \leq n
\end{aligned}
$$

(for $n$ large)

probability of error:

$$
\begin{aligned}
\mathbb{P}(\mathcal{S}_k \neq \mathcal{S}) &= \mathbb{P}\left(\{\mathcal{S}^c \cap \mathcal{S}_k \neq \emptyset\} \cup \{\mathcal{S} \cap \mathcal{S}_k^c \neq \emptyset\}\right) \\
&\leq \mathbb{P}\left(\mathcal{S}^c \cap \mathcal{S}_k \neq \emptyset\right) + \mathbb{P}\left(\mathcal{S} \cap \mathcal{S}_k^c \neq \emptyset\right)
\end{aligned}
$$

# False Positives

$$\mathbb{P}(\mathcal{S}_k \neq \mathcal{S}) \quad \leq \quad \mathbb{P}\left(\mathcal{S}^c \cap \mathcal{S}_k \neq \emptyset\right) \; + \; \mathbb{P}\left(\mathcal{S} \cap \mathcal{S}_k^c \neq \emptyset\right)$$

$$\begin{aligned}
\mathbb{P}\left(\mathcal{S}^c \cap \mathcal{S}_k \neq \emptyset\right) \quad &= \quad \mathbb{P}\left(\bigcup_{i \notin \mathcal{S}} \bigcap_{j=1}^{k} y_{i,j} > 0\right) \\
&\leq \quad \sum_{i \notin \mathcal{S}} \mathbb{P}\left(\bigcap_{j=1}^{k} y_{i,j} > 0\right) \\
&= \quad \sum_{i \notin \mathcal{S}} 2^{-k} \;=\; \frac{n-s}{2^k}
\end{aligned}$$

# False Negatives

$$\mathbb{P}(\mathcal{S}_k \neq \mathcal{S}) \quad \leq \quad \mathbb{P}\left(\mathcal{S}^c \cap \mathcal{S}_k \neq \emptyset\right) \; + \; \mathbb{P}\left(\mathcal{S} \cap \mathcal{S}_k^c \neq \emptyset\right)$$

$$\begin{aligned} \mathbb{P}\left(\mathcal{S} \cap \mathcal{S}_k^c \neq \emptyset\right) \quad &= \quad \mathbb{P}\left( \bigcup_{j=1}^{k} \bigcup_{i \in \mathcal{S}} y_{i,j} < 0 \right) \\ &\leq \quad \frac{k|\mathcal{S}|}{2} \, \exp\left( -\frac{\mu^2}{2(2+\epsilon)} \right) \end{aligned}$$

# Probability of Error Bound

$$
\begin{aligned}
\mathbb{P}(\mathcal{S}_k \neq \mathcal{S}) &\leq \mathbb{P}\left(\mathcal{S}^c \cap \mathcal{S}_k \neq \emptyset\right) + \mathbb{P}\left(\mathcal{S} \cap \mathcal{S}_k^c \neq \emptyset\right) \\
&\leq \frac{n-s}{2^k} + \frac{k|\mathcal{S}|}{2} \exp\left(-\frac{\mu^2}{2(2+\epsilon)}\right) \\
&= \frac{n-s}{2^k} + \frac{1}{2} \exp\left(-\frac{(\mu^2 - 2(2+\epsilon)\log(k|\mathcal{S}|))}{2(2+\epsilon)}\right)
\end{aligned}
$$

Consider high-dimensional limit as $n \to \infty$ and take $k = \log_2 n^{1+\epsilon}$

$$
\mathbb{P}(\mathcal{S}_k \neq \mathcal{S}) \leq \underbrace{\frac{n-s}{2^k}}_{\to 0} + \frac{1}{2} \exp\left(-\frac{(\mu^2 - 2(2+\epsilon)\log(|\mathcal{S}|(1+\epsilon)\log_2 n))}{2(2+\epsilon)}\right)
$$

Second term tends to zero if

$$
\mu \geq \sqrt{2(2+\epsilon)\log(|\mathcal{S}|(1+\epsilon)\log_2 n)}
$$

# Gains of Sequential Design

non-adaptive threshold:

$$\mu \;\geq\; \sqrt{2\log n}$$

DS threshold:

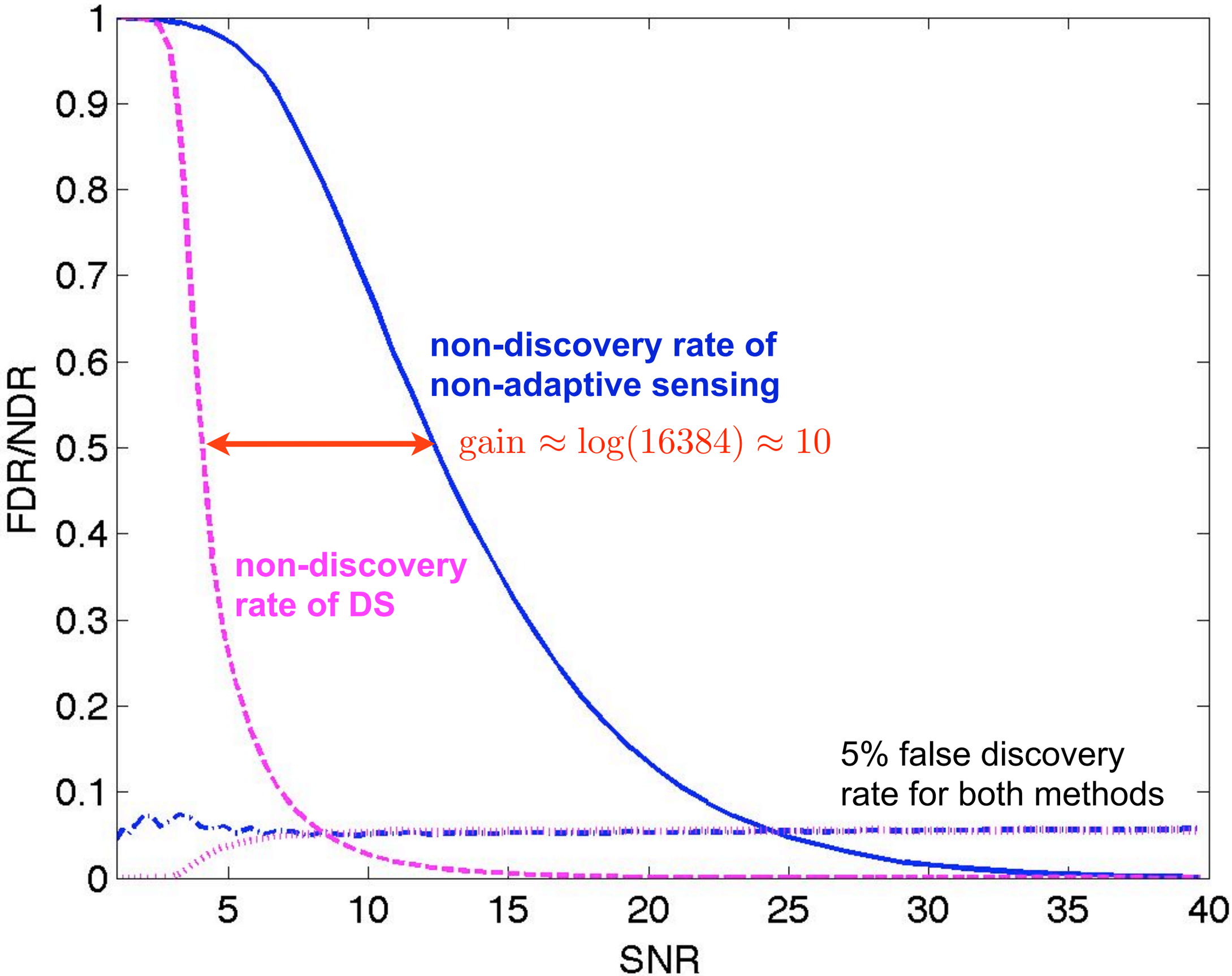
$$\begin{aligned}\mu &\geq \sqrt{2(2+\epsilon)\log(|\mathcal{S}|(1+\epsilon)\log_2 n)} \\ &\approx \sqrt{4\log|\mathcal{S}|}\end{aligned}$$

**We get a gain whenever $|\mathcal{S}| \preceq n^{1/2}$**

**Punchline:** In ultra-sparse setting, say $|\mathcal{S}| = C\log n$, DS drives error to zero if $\mu \geq \sqrt{(8+\epsilon)\log\log n}$, compared to the non-adaptive requirement $\mu \geq \sqrt{2\log n}$.

# Example

$n = 2^{14}, \ \|x\|_0 = \sqrt{n} = 128$



# Conclusions

## Sequential Experimental Designs for High-Dimensional Models

thresholds for recovery in high-dimensional limit:

| | |
|---|---|
| **non-adaptive designs** | $\text{SNR} \sim \log n$ |
| **sequential designs** | $\text{SNR} \sim$ arbitrarily slowly growing function of $n$ |

Distilled Sensing: Adaptive Sampling for Sparse Detection and Estimation
J. Haupt, R. Castro, and RN, **arXiv:1001.5311v2**

## Geometry of Sequential Inference

number of membership queries required to learn a set to $\epsilon$ accuracy:

| | |
|---|---|
| **non-adaptive** | $\#$ queries $\sim 1/\epsilon$ |
| **adaptive** | $\#$ queries $\sim \log(1/\epsilon)$ |

The Geometry of Generalized Binary Search, RN, **arXiv:0910.4397**