Graph Classification via Signal Subgraphs: Sex Classification from Human Connectomes

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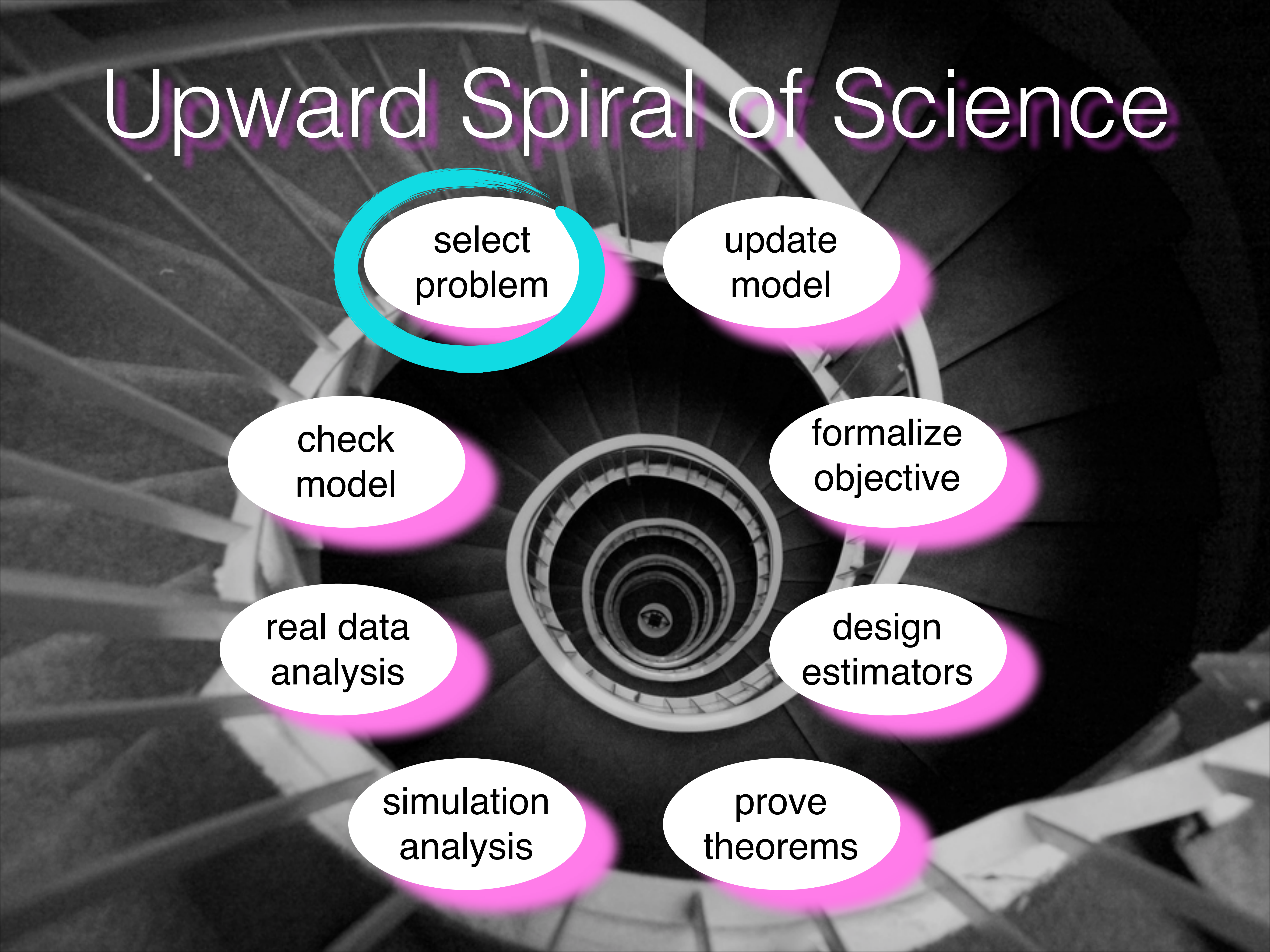
Upward Spiral of Science
select problem
update model
formalize objective
design estimators
prove theorems
simulation analysis
real data analysis
check model

Statistical Pattern Recognition

(for Big Scientific Data)

Problems	Methodologies	Desiderata
Hypothesis Testing	Parametric	(Asymptotic) Theory
Classification	Semi-Parametric	Robustness
Regression	Non-Parametric	*Non-Euclidean*
Density Estimation	Metric	*Low-D Structure*
Model Selection	Hacko-metric	Computational Speed
Clustering	Bayesian	Empirical Performance
Assignment	Optimization	Reproducible
Blind Deconvolution	Heuristic	Scalable

Statistical Pattern Recognition

This talk: Given $\{(G_i, Y_i)\}$, minimize $P[h(G) \neq Y]$

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Clinically Useful Biomarkers

APA Official Actions

Consensus Report of the APA Work Group on Neuroimaging Markers of Psychiatric Disorders
RESOURCE DOCUMENT

introduction to this paper, there are currently no brain imaging biomarkers that are currently clinically useful for any diagnostic category in psychiatry.

Mental Illness in USA

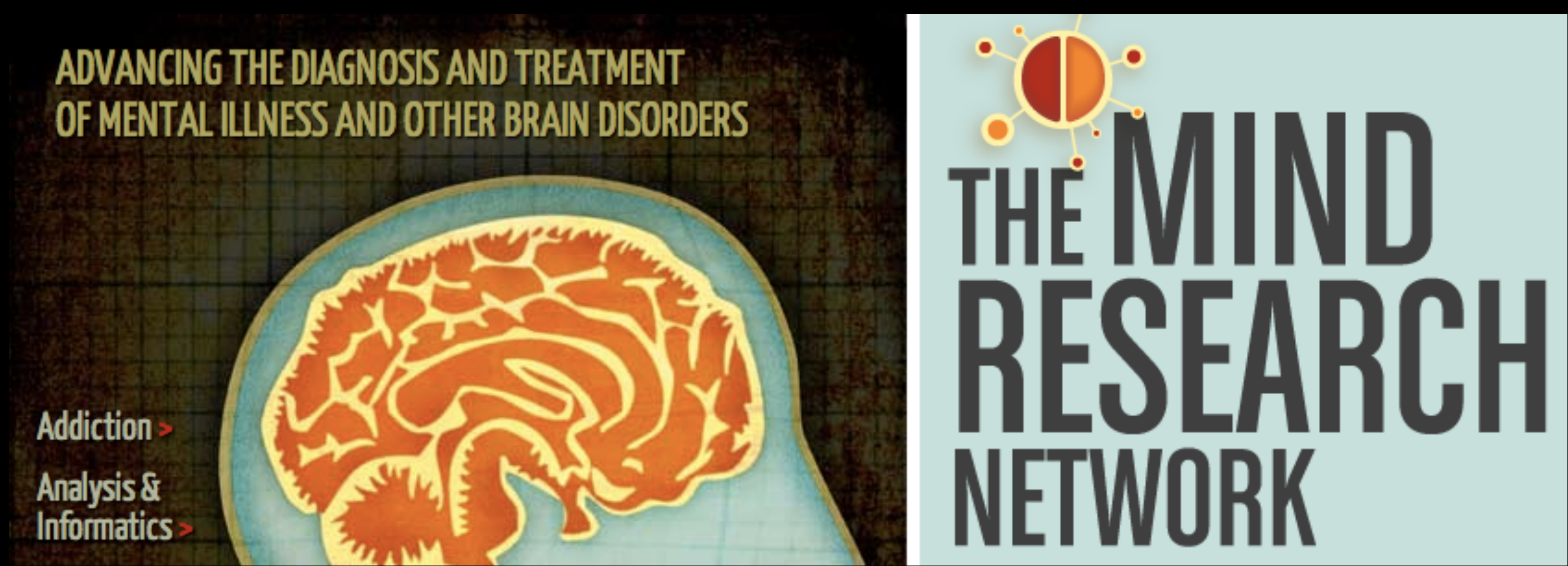
% Affected	Impact
100% people have brains	~$200B / yr
25% / year	3rd most common cause of hospitalization
20% prisoners recent	>50% drop-out
20% youths severe	suicide is the 10th leading cause of death
70% juvenile prisoners	#'s are increasing quickly

Connectomes

Datasets Popping Up

Human Connectome Project

Home | About | Data | Informatics | Gallery | Publications | News



The MGH Superstruct Project

Creating a World Class Resource for Psychiatric Neuroscience

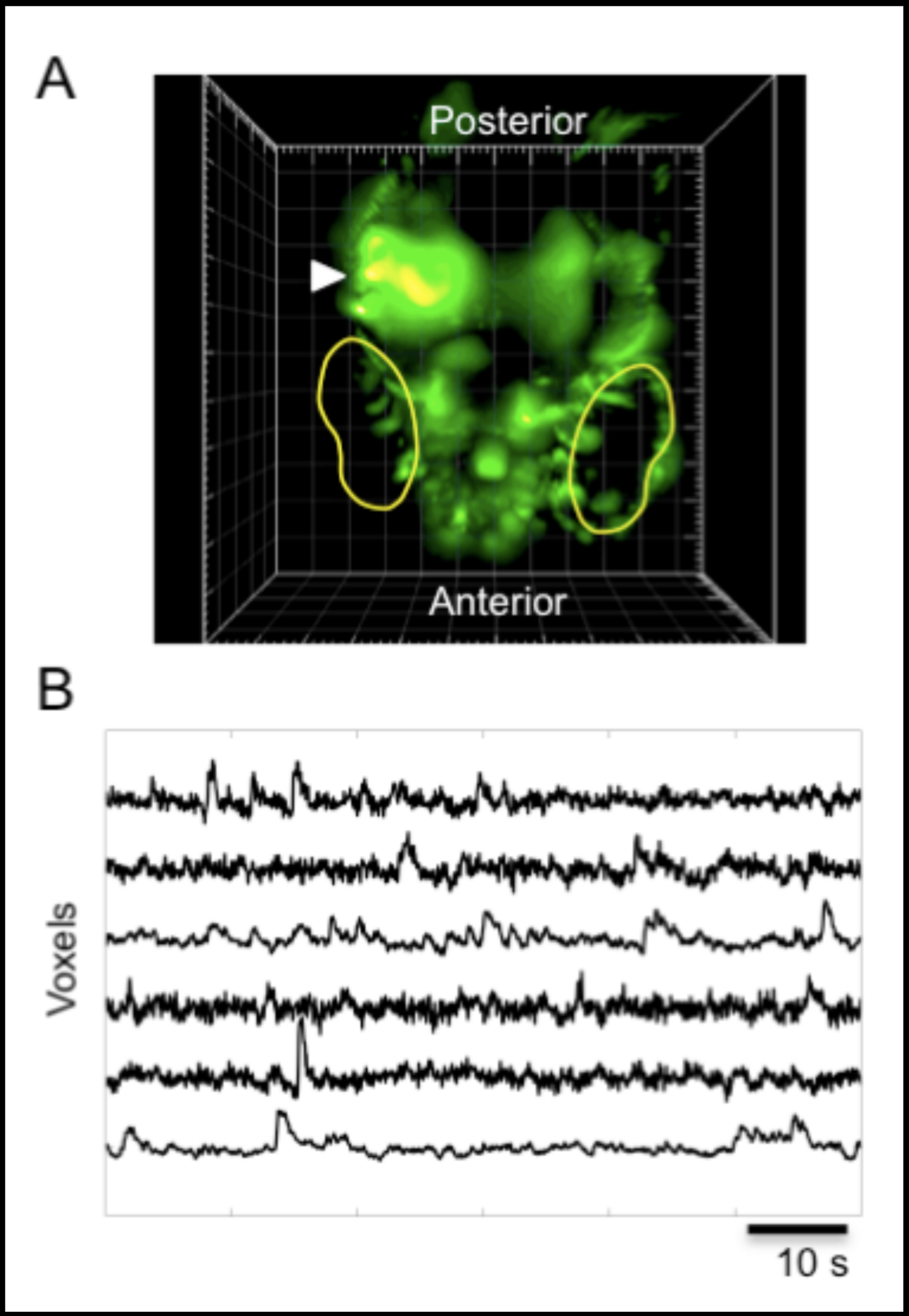
One of the great discoveries of modern science is that thought, feeling and behavior consist of physiological activity in the brain. Through the neuroimaging revolution of the 1990s, images of activity in the thinking brain are a familiar sight. A second revolution, occurring over the last decade, is genomics, the study of DNA and RNA sequences of the human genome.

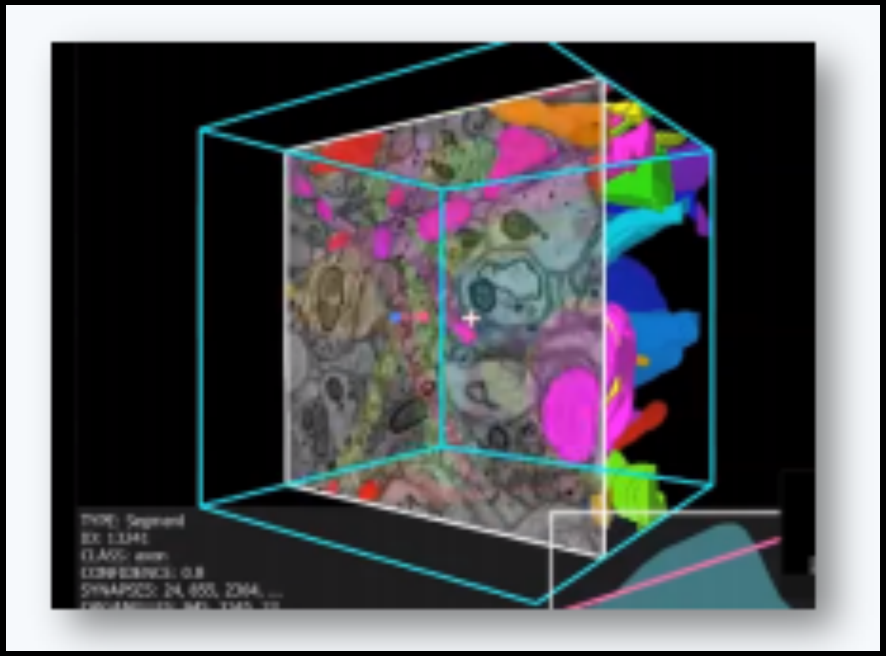
1000 FUNCTIONAL CONNECTOMES PROJECT

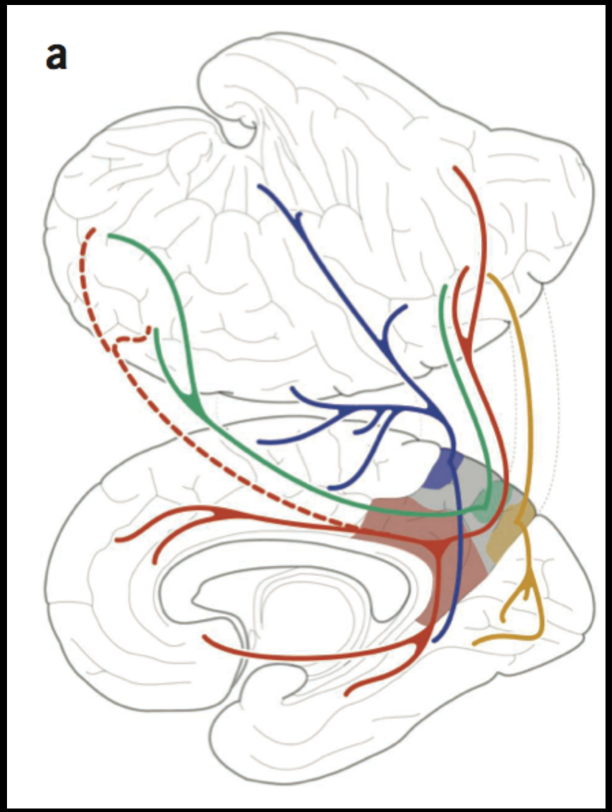
indi

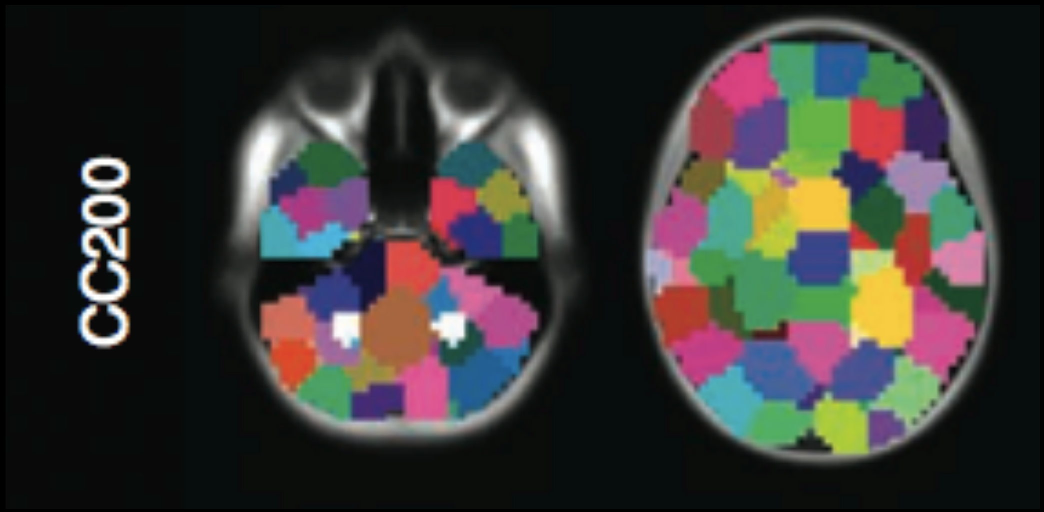
International Neuroimaging Data-Sharing Initiative

Graph Inference





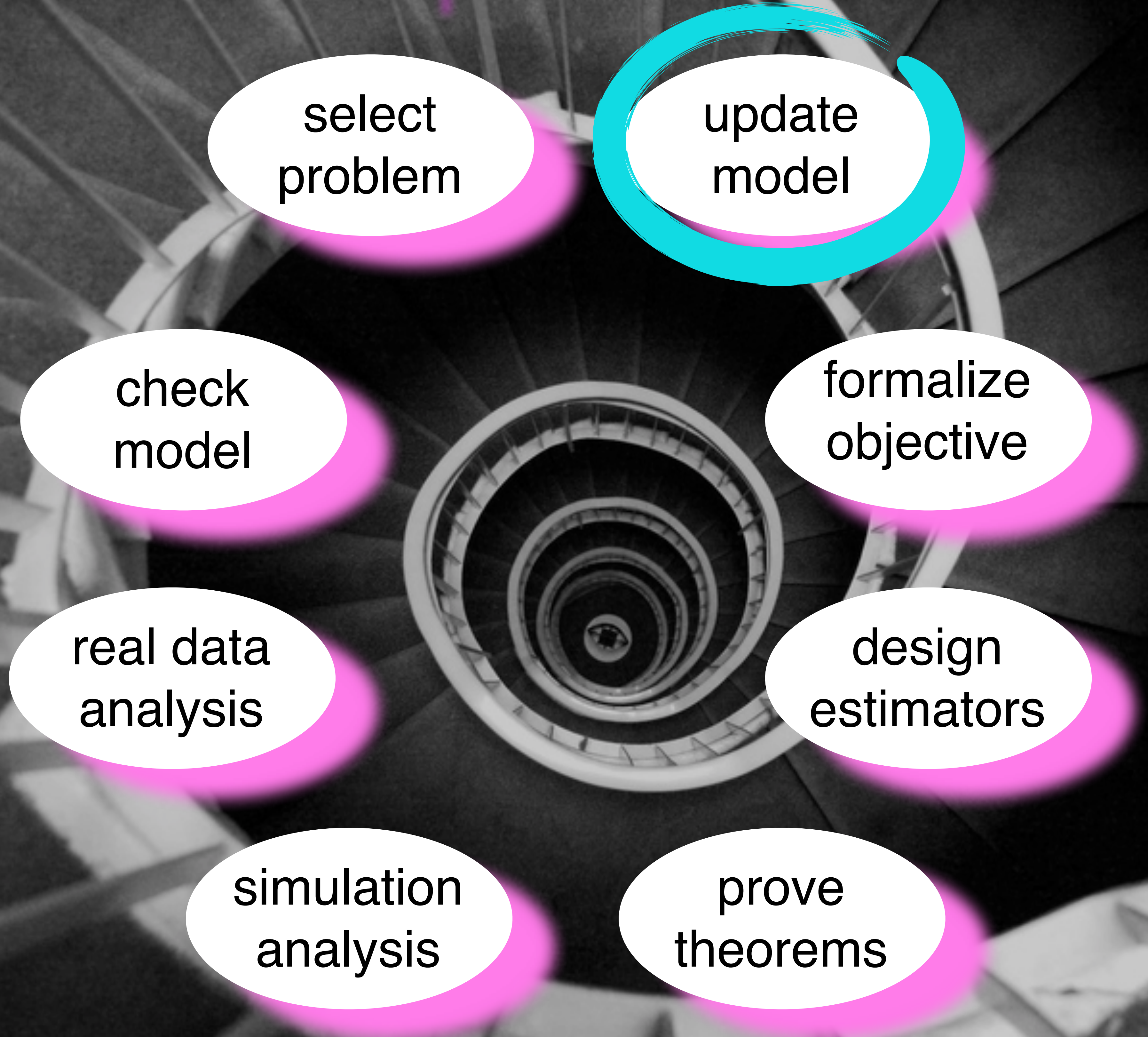




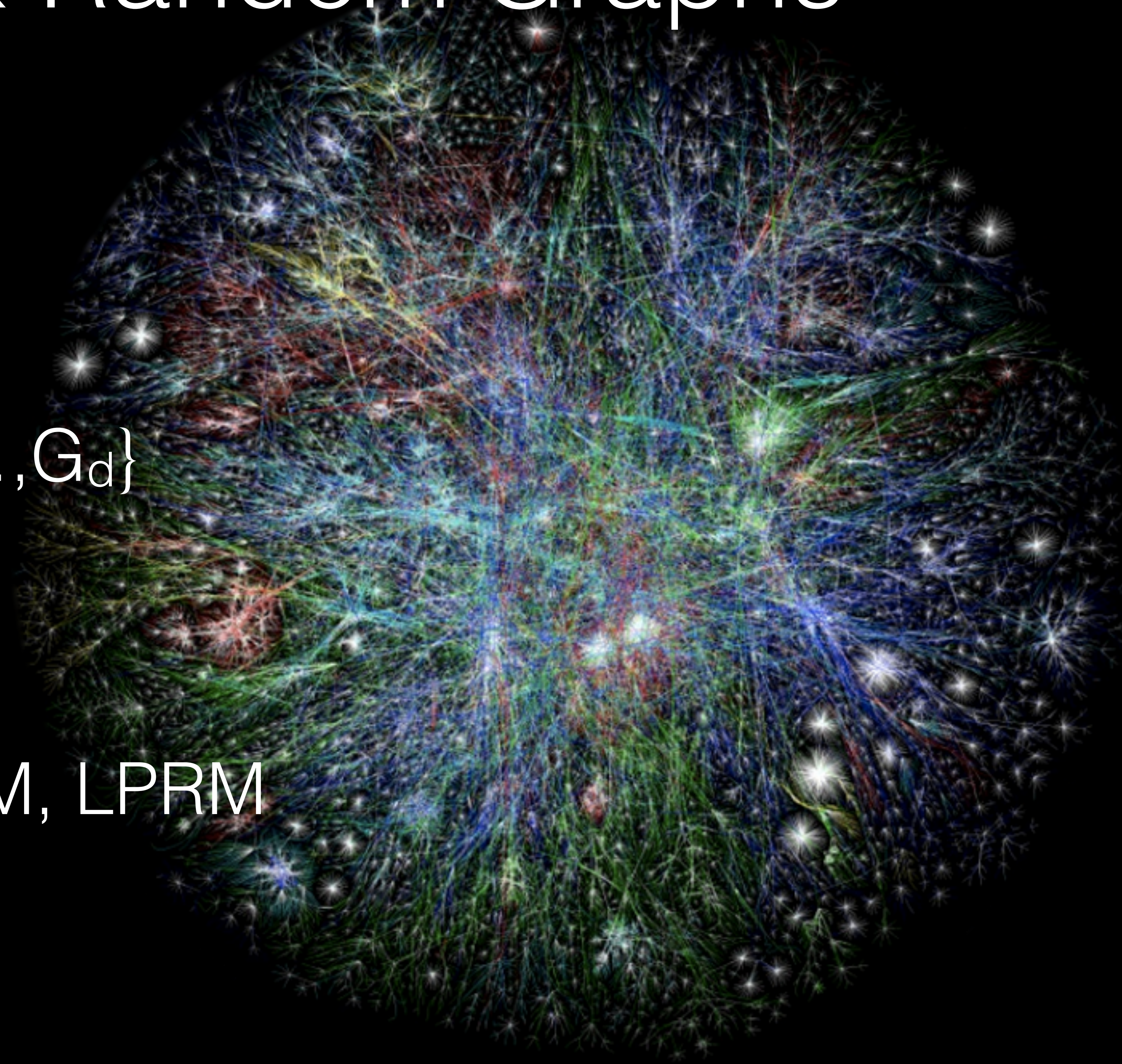
Summary of Problem Selection

- Open problems in Statistics of Graphs
- Pressing societal issue
- No suitable methods available
- Data are available

Upward Spiral of Science



Update Model:
Graphs & Random Graphs



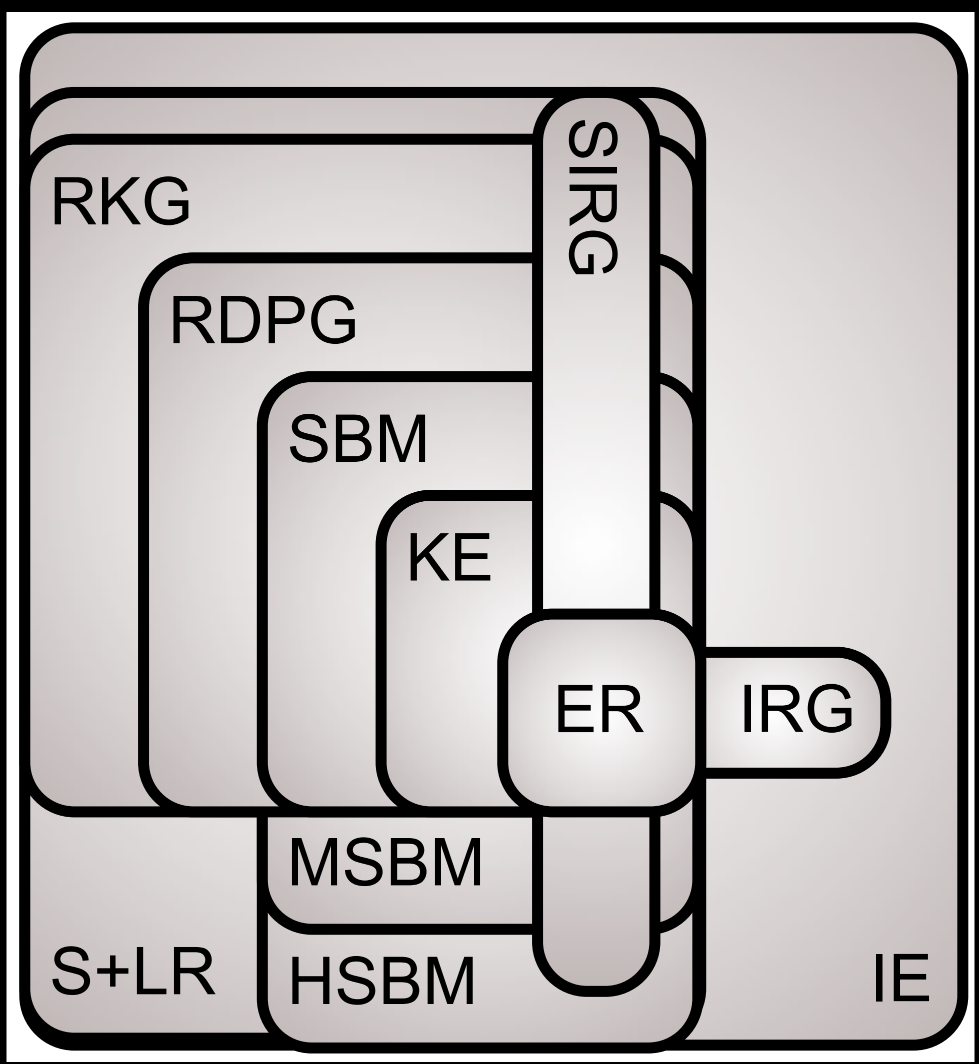
- $G=(V,E)$
- $\mathbf{G}: \boldsymbol{\Omega} \rightarrow \mathcal{G} = \{G_1,\ldots,G_d\}$
- $\mathbf{G} \sim F_G \in \mathcal{F}$
- e.g. $\mathcal{F}$'s: ER, ERGM, LPRM

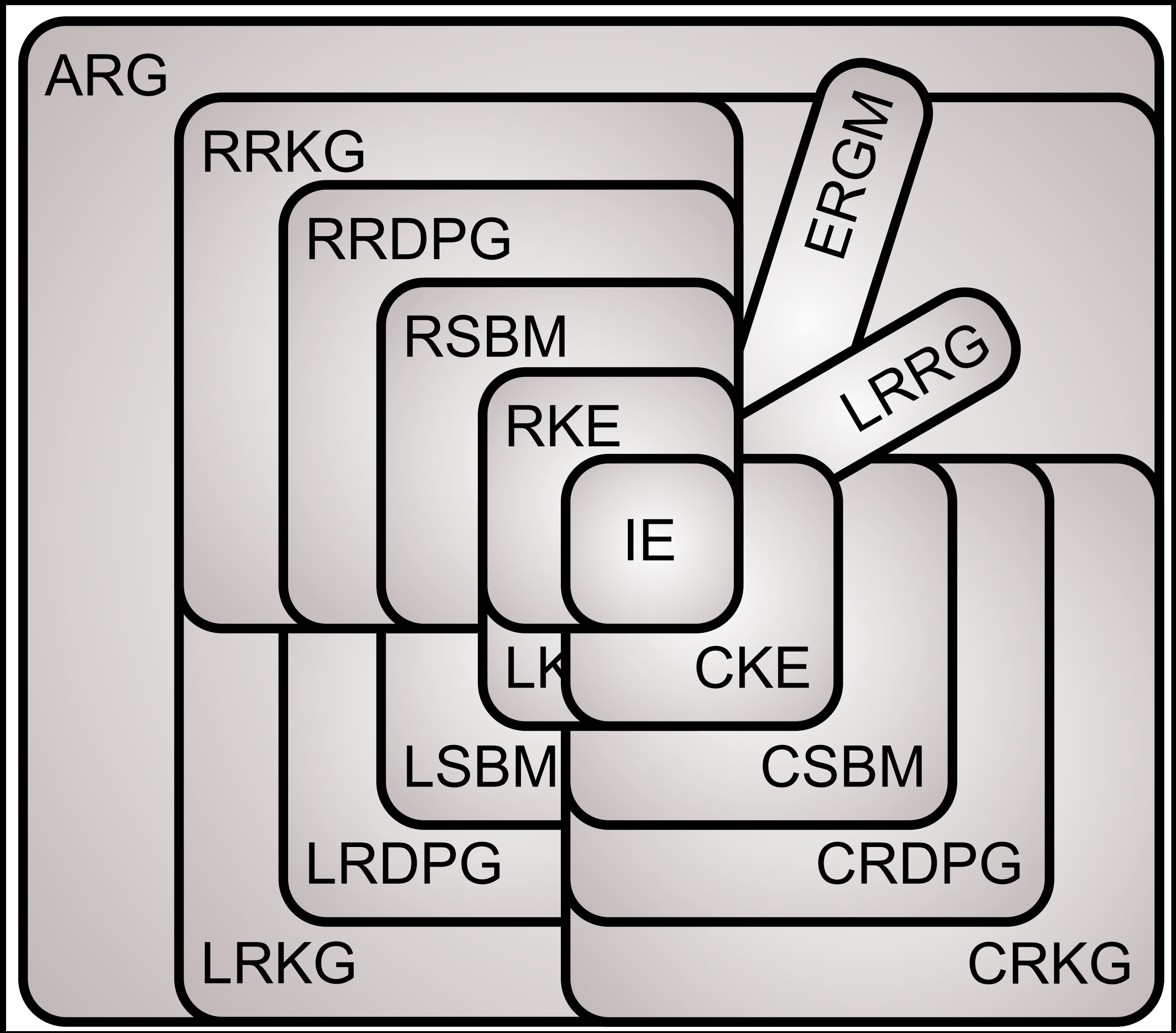
Update Model:
Consider the exploitation task

- $(G_i, Y_i) \sim F_{GY}$, $i \in \{1,\ldots,49\}$
- $G_i = (V, E_i)$, where $|V|=70$
- $Y_i \in \{0,1\}$, $n_0 = 25$, $n_1 = 24$
- Objective: classify and find signal subgraph

Update Model:
Random Graph Complexity Zoo

Trading off expressiveness with estimability



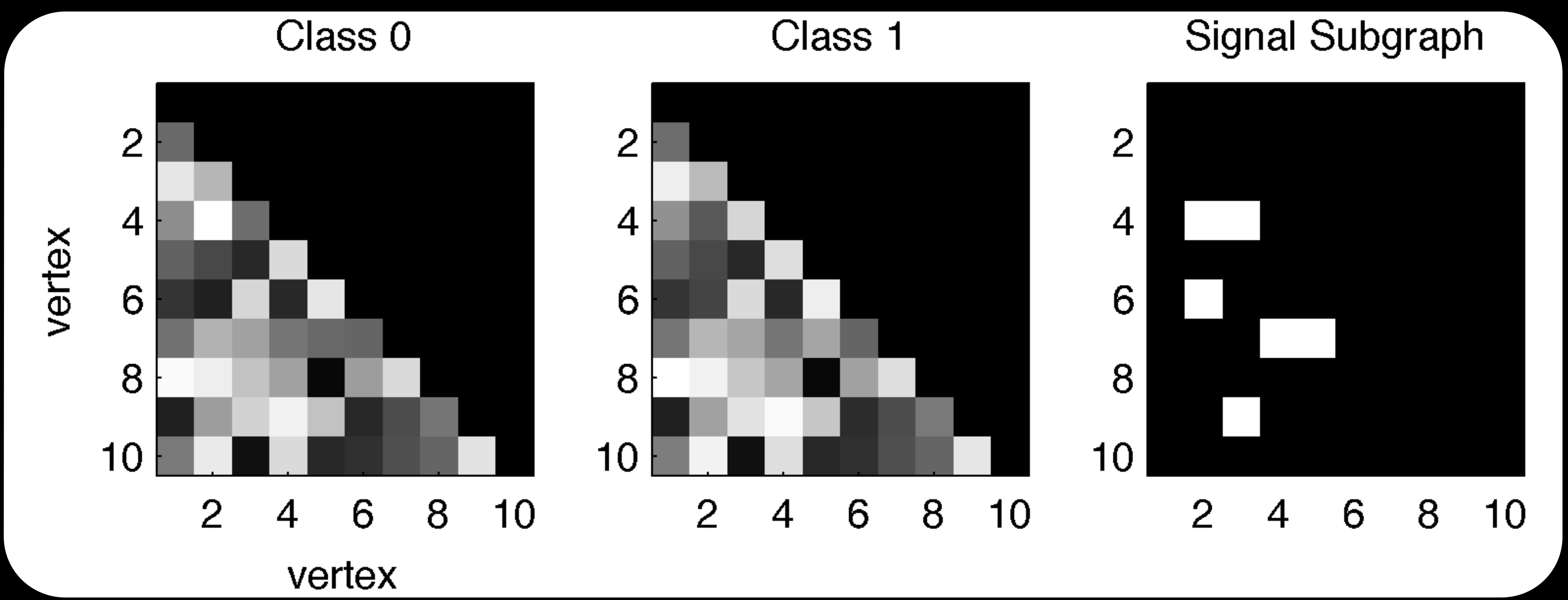


Update Model:
Signal Subgraph Model

1. all graphs have the same set of labeled vertices

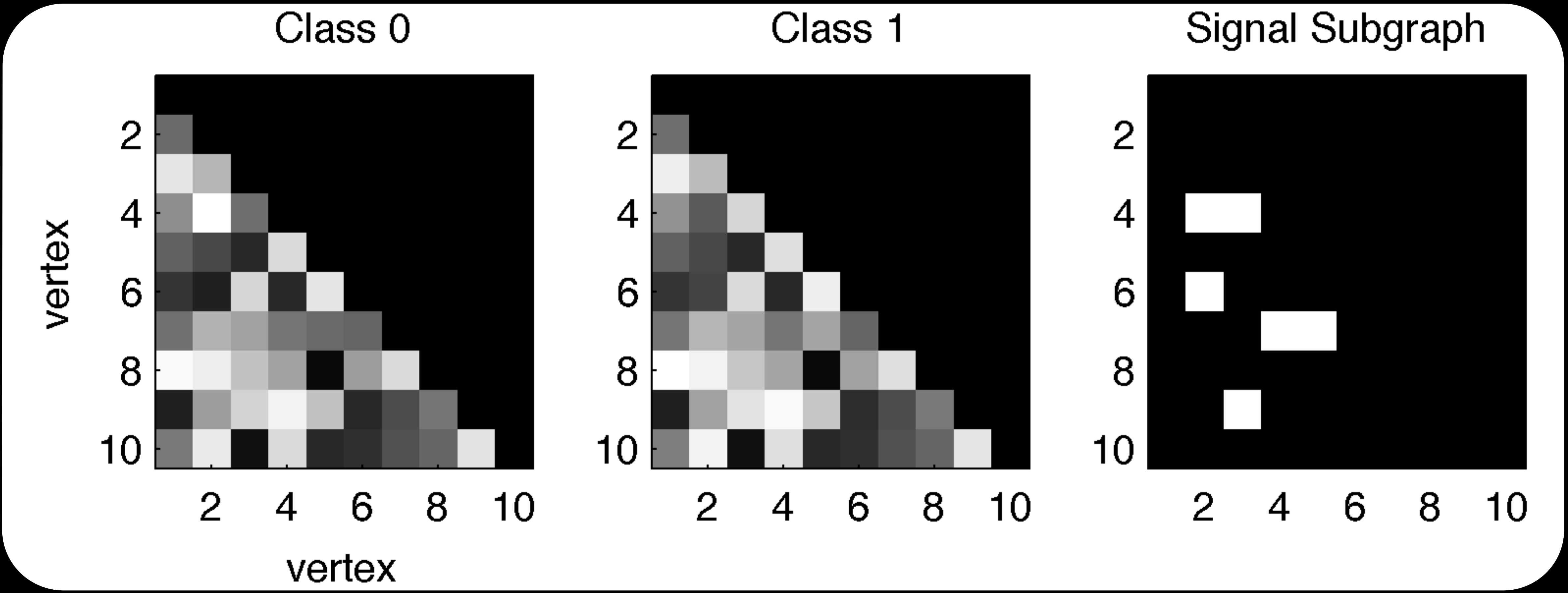
2. edges are sampled independently

3. only a subset of edges contain any class conditional signal



Update Model:
Signal Subgraph Model

1. $F_{G|Y} = F_{A|Y}$
2. $F_{A|Y} = \prod_{u,v} \mathrm{Bern}(a_{uv}; \eta_{uv|y})$
3. $F_{A|Y} = \prod_{u,v \in S} \mathrm{Bern}(a_{uv}; \eta_{uv|y}) \times \prod_{uv \notin S} \mathrm{Bern}(a_{uv}; \eta_{uv})$



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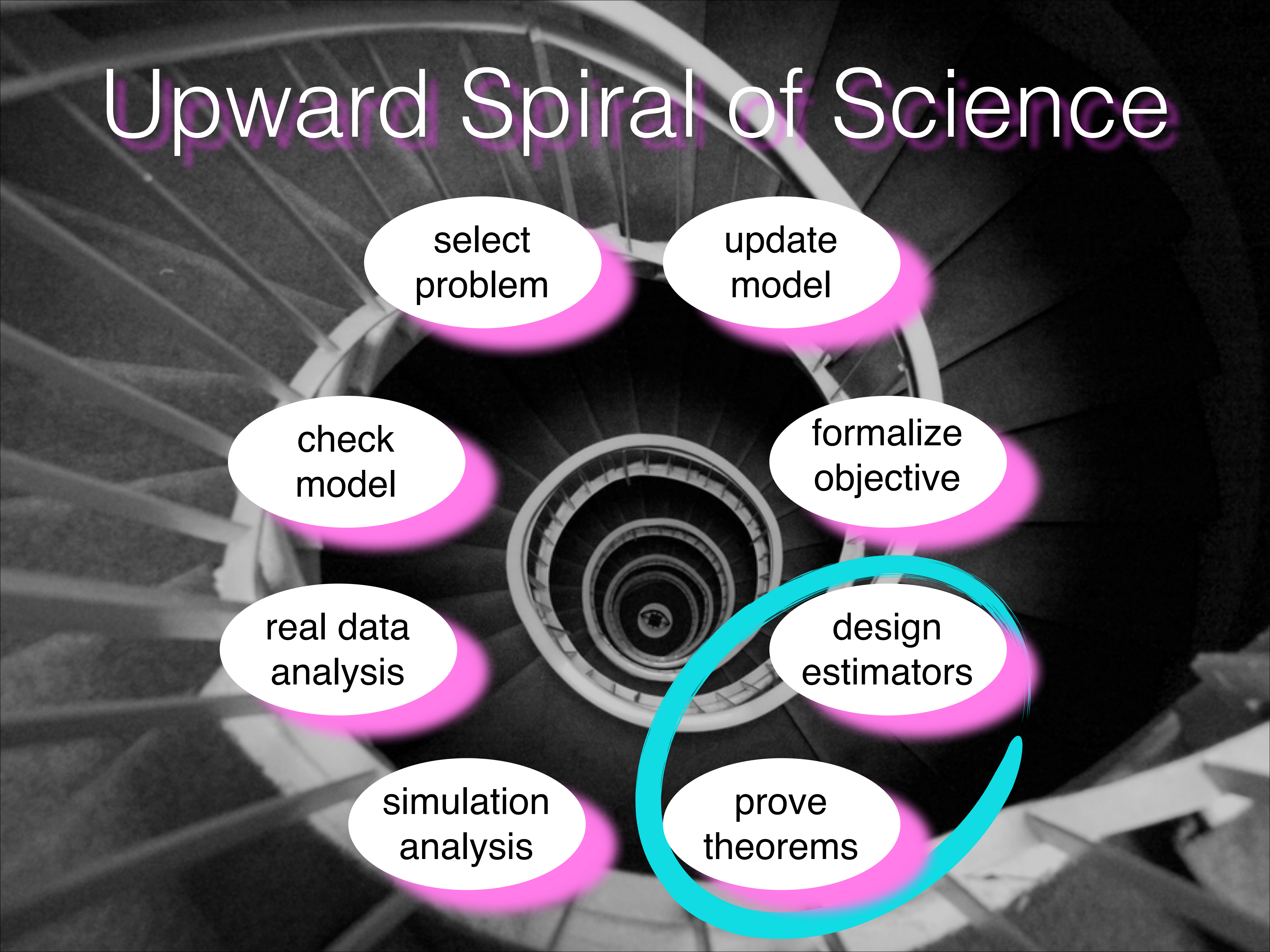
Formalize Objective
Graph Classification

- (**G,Y**) ~ F_{GY} ϵ $\mathcal{F}$
- find h(**G**), s.t. P[h(**G**)≠**Y**] is minimized
- if we knew F_{GY}, we could use the Bayes classifier:
  - $h^*(G) := \text{argmax}_Y F_{Y|G} = \text{argmax}_Y F_{G|Y} F_Y$
- since we don't know F_{GY}, we instead consider the Bayes plug-in
  - $h_n G) := \text{argmax}_Y F'_{Y|G} = \text{argmax}_Y F'_{G|Y} F'_Y$
  - where F' indicates an estimate of F

Formalize Objective
Graph Classification

- $F_{A|Y}F_Y = \mathrm{Bern}(y;p') \prod_{u,v \in S'} \mathrm{Bern}(a_{uv}; \eta'_{uv|y}) \times \prod_{uv \notin S'} \mathrm{Bern}(a_{uv}; \eta'_{uv})$
- $F_{A|Y}F_Y = \mathrm{Bern}(y;p') \prod_{u,v \in S'} \mathrm{Bern}(a_{uv}; \eta'_{uv|y})$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Design Estimator
Plug-in Classifier Procedure

1. estimate prior parameter
2. estimate class-conditional likelihood parameters
3. estimate signal subgraph
4. plug-in those badboys

Design Estimator
1. Estimating the Prior

trivial! the maximum likelihood estimate (MLE) suffices:

$$\hat{\pi}_y = \sum_{i \in [n]} \frac{\mathbb{I}\{y_i = y\}}{n}$$

Design Estimator
2. Estimating the Likelihood

- MLE does not suffice
- it is sometimes 0 or 1; boundaries are evil.
- MAP with “non-informative prior” doesn’t help

Design Estimator

2. Robust Estimator of the Likelihood

$$\hat{\eta}_{uv|y} = \begin{cases} \epsilon_n & \text{if } \max_{i:y_i=y} a_{uv}^{(i)} = 0 \\ 1-\epsilon_n & \text{if } \min_{i:y_i=y} a_{uv}^{(i)} = 1 \\ \hat{\eta}_{uv|y}^{MLE} & \text{otherwise} \end{cases}$$

$$\epsilon_n = 1/(10n)$$

Thm 1: consistent to MLE as n increases

Proof: it is an L-estimator (c.f., Huber, '04)

Design Estimator
2. Proof of Robustness

L-estimator: a linear combination of (nonlinear functions of) order statistics

$$T_n = \sum_{i=1}^{n} a_{ni} h(x_{(i)}).$$

$$h(x^{(i)}) = \begin{cases} \epsilon_n & \text{if } \max\limits_{i:y_i=y} a_{uv}^{(i)} = 0 \\ 1-\epsilon_n & \text{if } \min\limits_{i:y_i=y} a_{uv}^{(i)} = 1 \\ x^{(i)} & \text{otherwise} \end{cases}$$

$$a_{ni} = 1/n$$

Design Estimator
3. Estimating the Signal Subgraph

$$\begin{aligned}
\text{Signal subgraph: } & \mathcal{S} = \{u \sim v : \eta_{uv|y} \neq \eta_{uv|y'}\} \\
\text{Signal vertices: } & \mathcal{V} = \arg\min_{V'} V' \\
& V' = \{v : \forall u \sim v \in \mathcal{S}, u \cup v \in V'\}
\end{aligned}$$

$$\begin{aligned}
\text{Incoherent Strategy: } & \text{Assume } |\mathcal{S}| = s \ll n^2 \text{ is known} \\
\text{Coherent Strategy: } & \text{Assume } |\mathcal{V}| = m \ll n \text{ is known}
\end{aligned}$$

Design Estimator
3. Incoherent Estimator of Signal

- compute test statistic for each edge (e.g., Fisher's Exact test)
- the s most significant edges comprise the signal subgraph
- Thm 2: $\hat{\mathcal{S}}_{inc} \to \mathcal{S}$ as $n \to \infty$
- Proof: p-values converge to 0 for all edges in signal subgraph
- NB: some might call this "sparse"

Design Estimator

3. Procedure for Coherent Signal Estimate

1. compute the significance, T_{uv}, for each edge

2. rank-order edges by significance per vertex, $T_{k,(1)} \leq \cdots \leq T_{k,(n-1)}$

3. for $c = T_{(1)}, \ldots T_{(d)}$

   (a) score each vertex according to how many edges incident to it are significant, $w_{v;c} = \sum_u \mathbb{I}\{T_{uv} < c\}$

   (b) if $\sum_{v \in [m]} w_{v;c} \geq s$, break

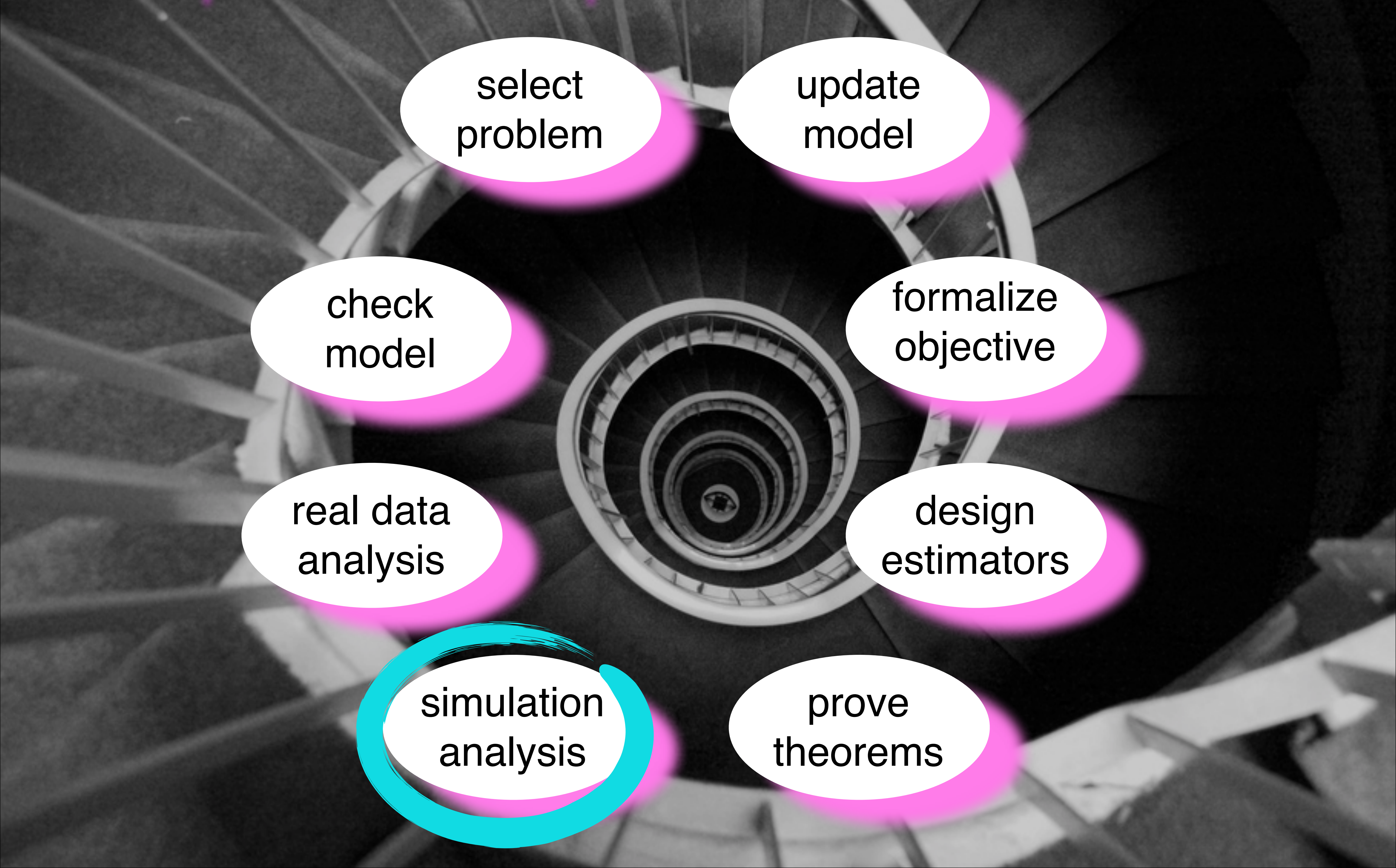
4. $\hat{S}_{con}$ are the s most significant edges of that subset

Design Estimator

3. Coherent Signal Estimate

- Thm 3: $\hat{\mathcal{S}}_{coh} \to \mathcal{S}$ as $n \to \infty$
- Proof: p-values converge to 0 for all edges in signal subgraph
- Conjecture 1: convergence rate is faster for coherent than incoherent under suitable conditions
- Conjecture 2: classification accuracy converges faster too
- NB1: some might call this “sparse & structured”
- NB2: this is a locally low-rank estimator

Upward Spiral of Science



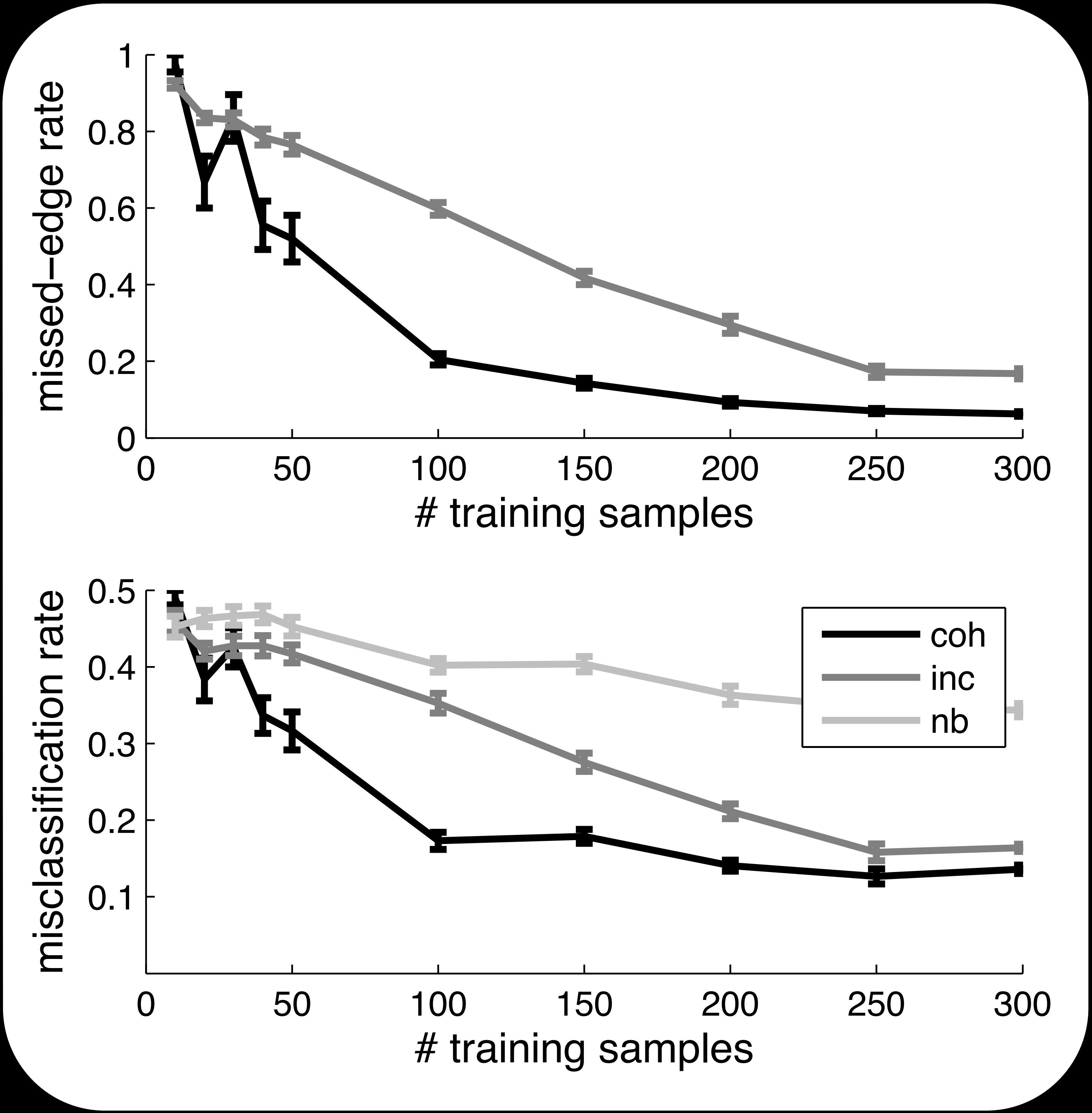
Sex Classification

Classifier	Error (%)
Naive Bayes	41
Lasso	27
Incoherent	27
Coherent	**16**
kNN	20
hacko-metric	**16**
Semi-parametric	**16**

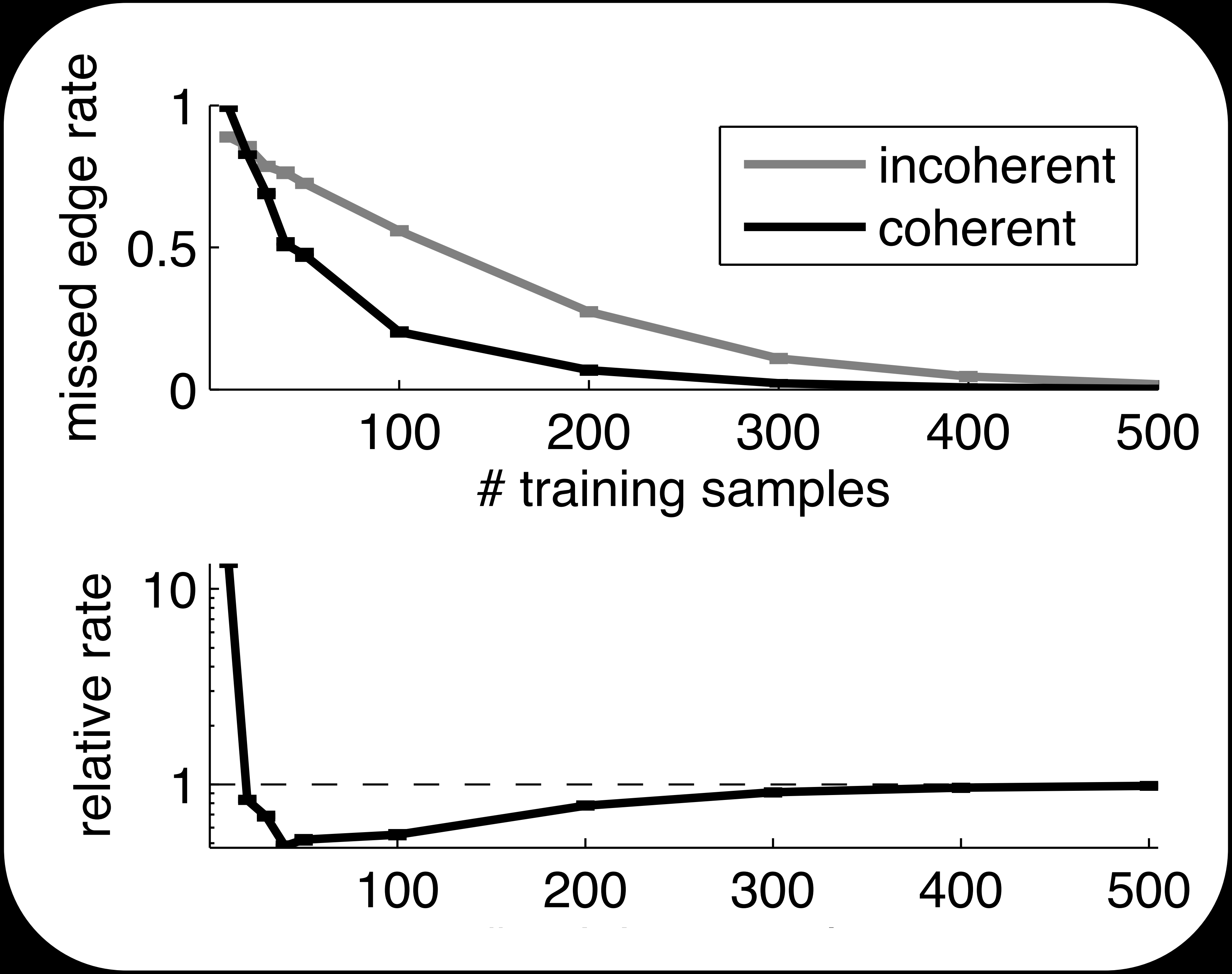
Numerical Analysis Simulated Data

1. Set $\{\eta_{uv|y}\}$ and $\{\pi_y\}$ and $|\mathcal{S}| = 20$ and $|\mathcal{V}| = 1$
2. for $i = 1, \ldots, n$, $y^i \sim \text{Bernoulli}(y; \pi_y)$
3. for $u, v = 1, \ldots, n$, $a^i_{uv}|y^i \sim \text{Bernoulli}(a_{uv}; \eta_{uv|y})$
4. estimate parameters using both strategies
5. compare edge selection and classification performance

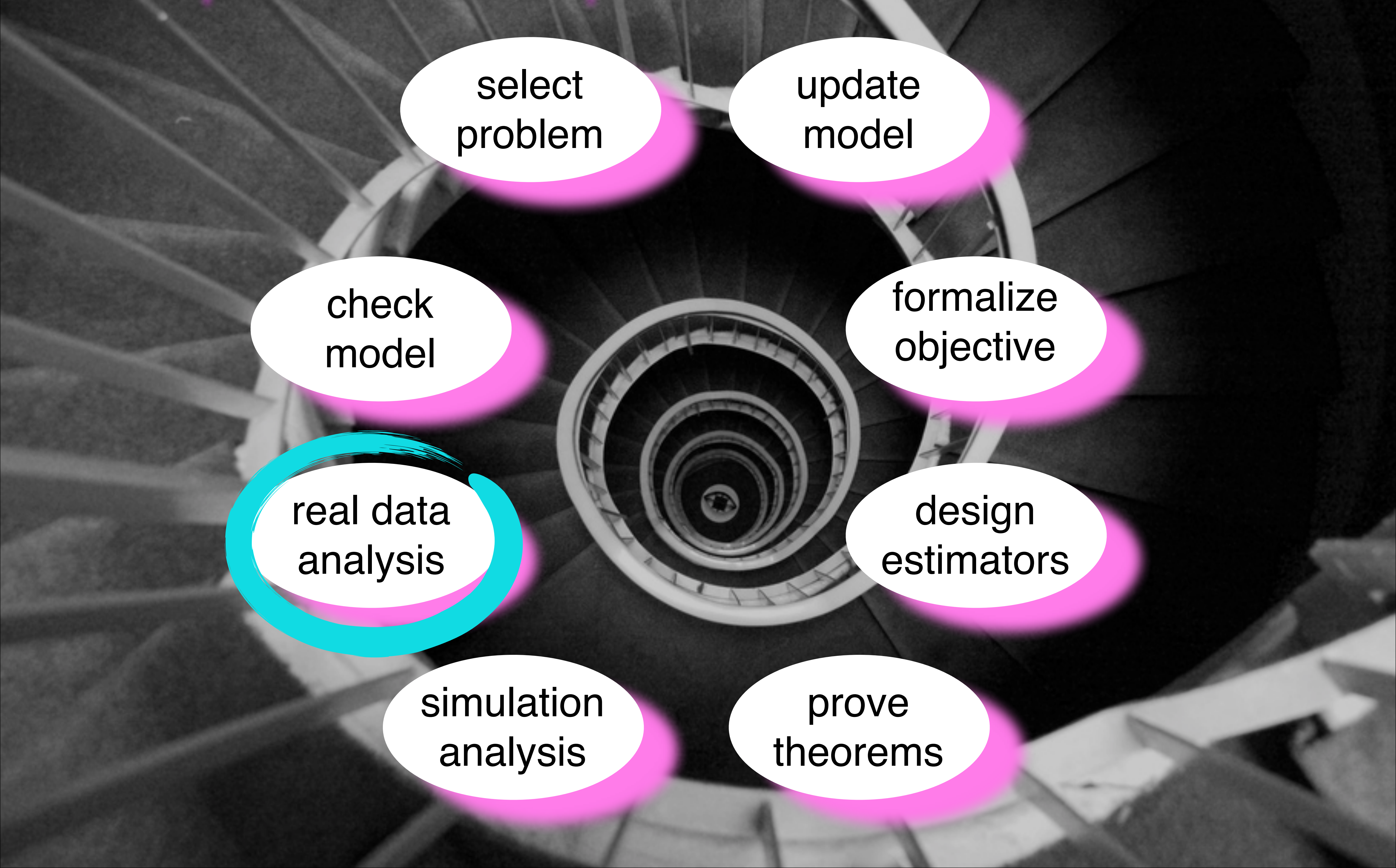
Simulated Data Analysis
Numerical Convergence



Simulated Data Analysis
Relative Efficiency



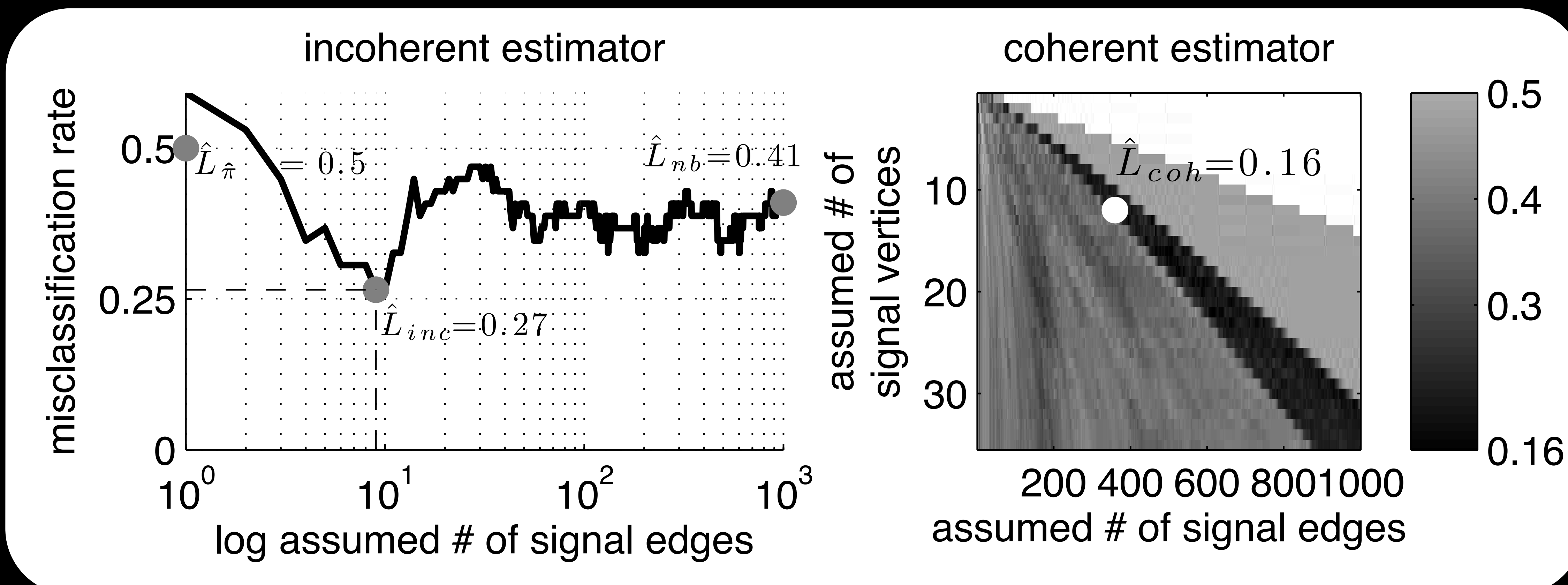
Upward Spiral of Science



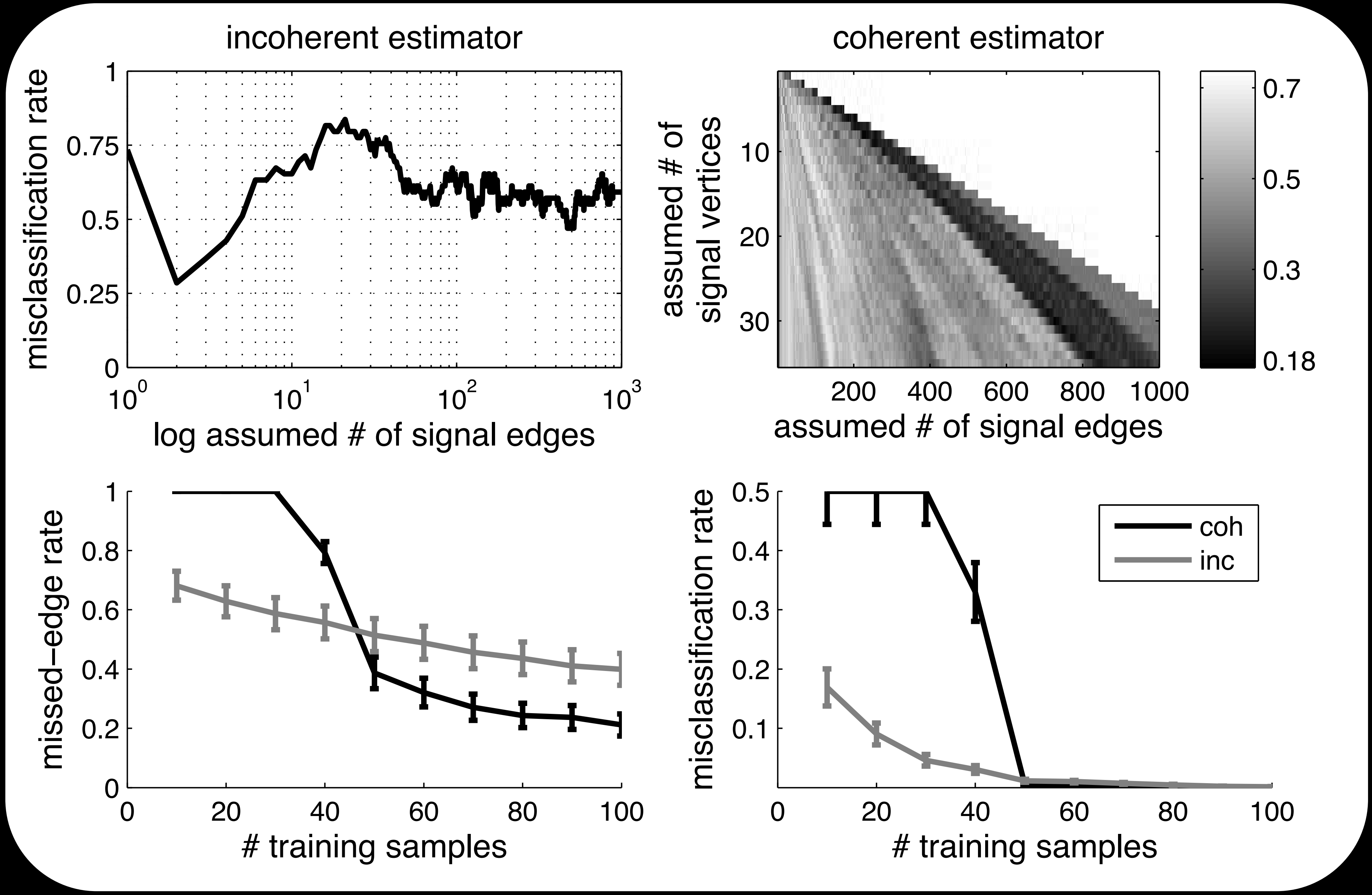
Real Data Analysis
Sex Classification

- Estimate brain-graphs from diffusion MRI
- Each graph has 70 labeled vertices (ROIs)
- 25 (24) male (female) subjects
- Objective: classify and find signal subgraph

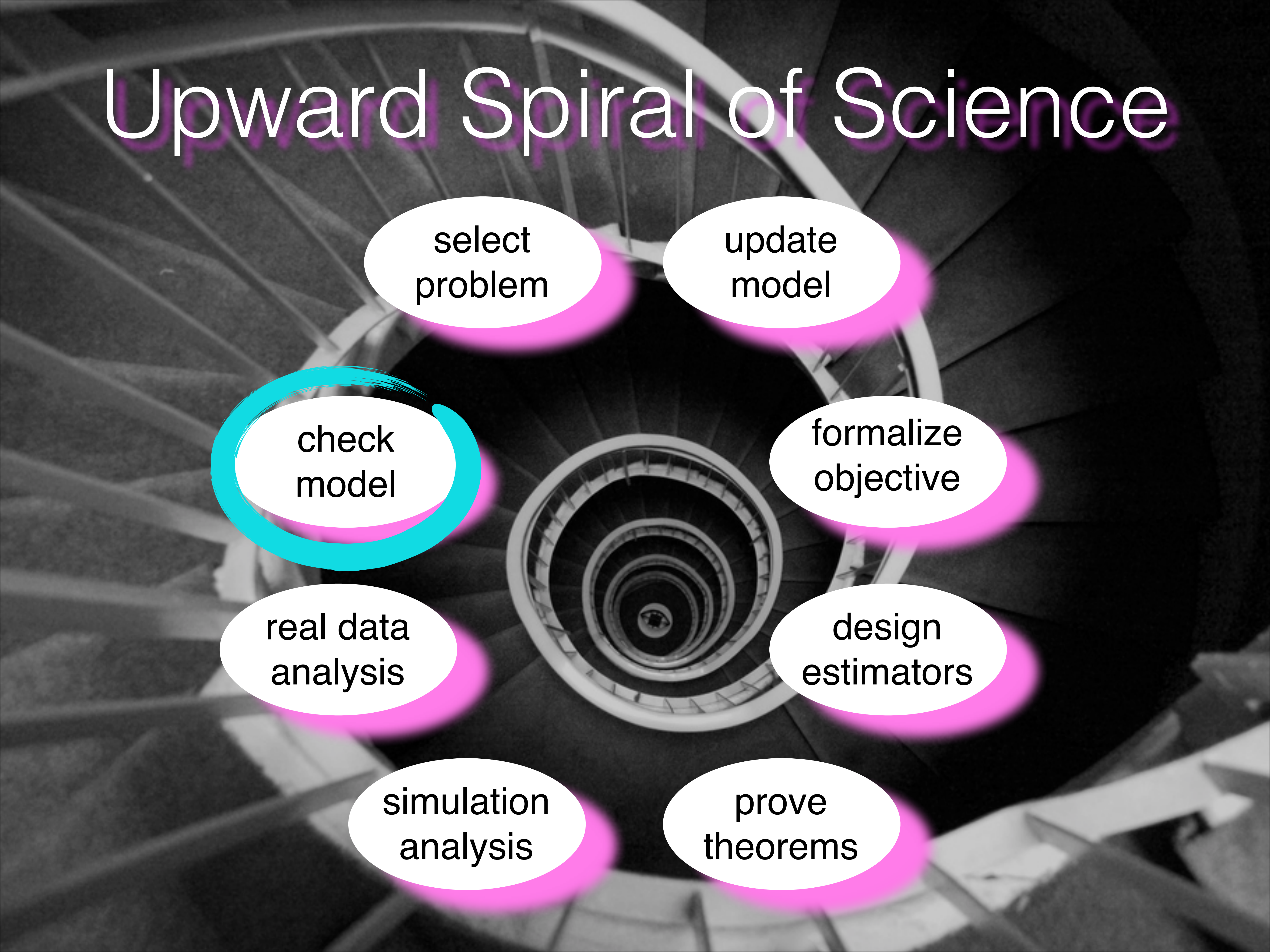
Real Data Analysis
LOOCV Performance



Real Data Analysis
Synthetic Data Analysis

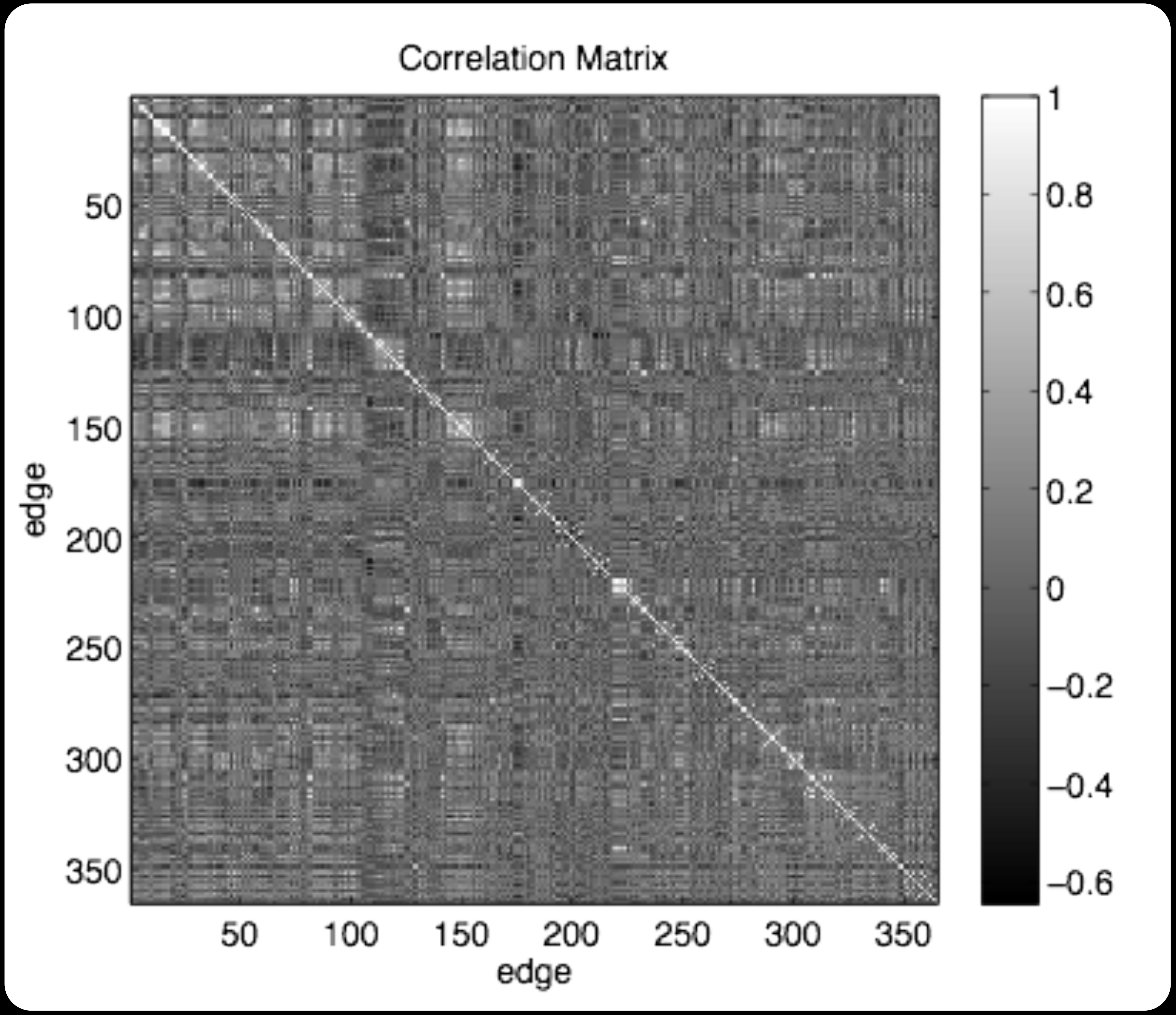


Upward Spiral of Science



Human Connectome

Model Checking



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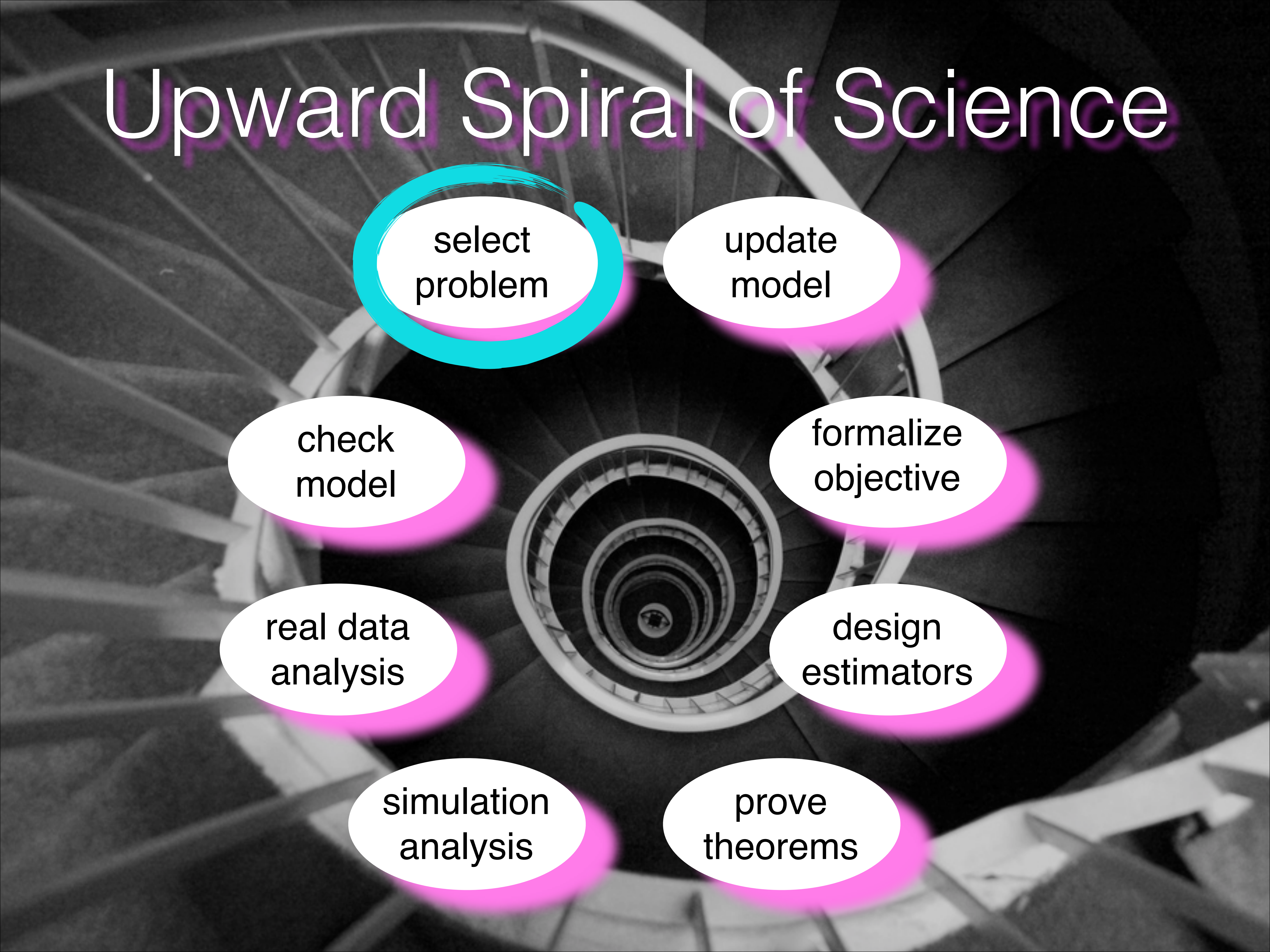

Statistical Pattern Recognition

This talk: Given $\{(G_i, Y_i)\}$, minimize $P[h(G) \neq Y]$

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Statistical Pattern Recognition

Other work: Given $\{(G_i,Y_i)\}$, minimize $P[h(G)\neq Y]$

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Statistical Pattern Recognition

Other work: Given G_1, G_2, minimize $\| G_1 - PG_2P' \|$

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Statistical Pattern Recognition

Other work: Given G~F, estimate F

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Assignment	Optimization	**Reproducible**
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Statistical Pattern Recognition

Other work: density estimation, deconvolution, etc.

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Regression	**Non-Parametric**	*Non-Euclidean*
Density Estimation	Metric	***Low-D Structure***
Model Selection	Hacko-metric	**Computational Speed**
Clustering	**Bayesian**	**Empirical Performance**
Assignment Problems	**Optimization**	**Reproducible**
Blind Deconvolution	Heuristic	**Scalable**

Future work:
Statistical Pattern Recognition for Graphs

Problems	Methodologies	Desiderata
Hypothesis Testing	**Parametric**	**(Asymptotic) Theory**
Classification	**Semi-Parametric**	**Robustness**
Regression	**Non-Parametric**	***Non-Euclidean***
Density Estimation	**Metric**	***Low-D Structure***
Model Selection	**Hacko-metric**	**Computational Speed**
Clustering	**Bayesian**	**Empirical Performance**
Assignment	**Optimization**	**Reproducible**
Blind Deconvolution	**Heuristic**	**Scalable**

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