Preprocessing, Multiphase Inference, and Massive Data in Theory and Practice

Alexander W Blocker

Department of Statistics
Harvard University

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Joint work with Xiao-Li Meng

Outline

Defining preprocessing

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- Widely considered an art, domain knowledge driven
- Aim to enhance domain knowledge with formal, mathematical theory

Perils and promise

Destructive preprocessing

- Most non-trivial preprocessing is irreversible
- Assumptions matter — and the wrong ones cause a lot of damage
- Preprocessing decisions constrain all later analyses, no matter the scale

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Alleviating complexity

- Smaller data and less complex modeling required
- Separation of effort among analysts (e.g. pipelines and workflows)

Massive data

Scale is not always a savior

- First step: preprocess and extract features
- If information is discarded or distorted by preprocessing, scale will not always save you
- Conversely, simple and huge with good preprocessing often beats complex

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Systematic errors at scale

- With massive data, systematic errors dominate statistical noise (e.g. Szalay)
- Observation/sensor models are vital (e.g. Ré)
- Help or harm depends on what is passed forwards

Theory vs. practice

Statistical theory

- Model generative process for observed data
- Evaluate procedures in their entirety

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Statistical practice

- Delineate between pre- and post-modeling work
- Formal evaluation only after preprocessing

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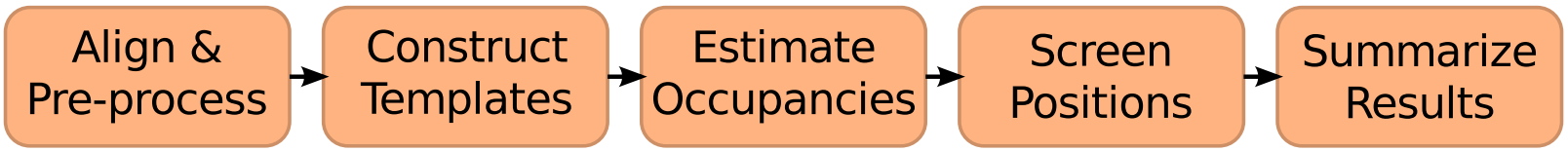
Closing the gap

- Want theoretical foundations for statistical practice
- Building this under banner of **multiphase inference** from theory of missing data

Multiphase, graphically



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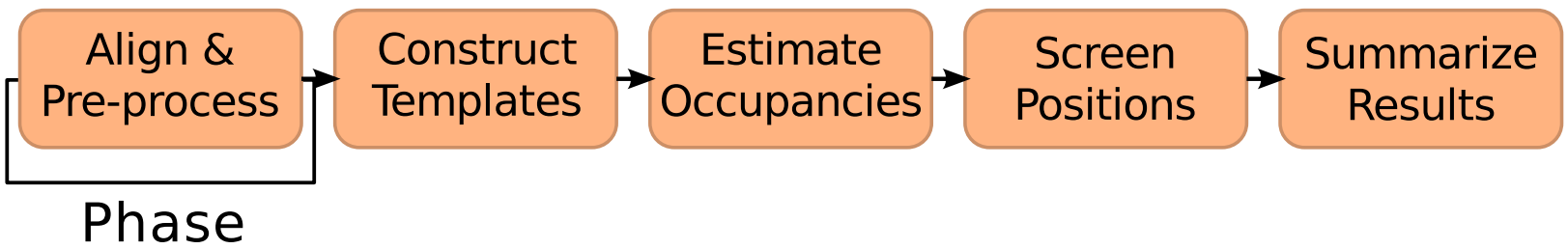

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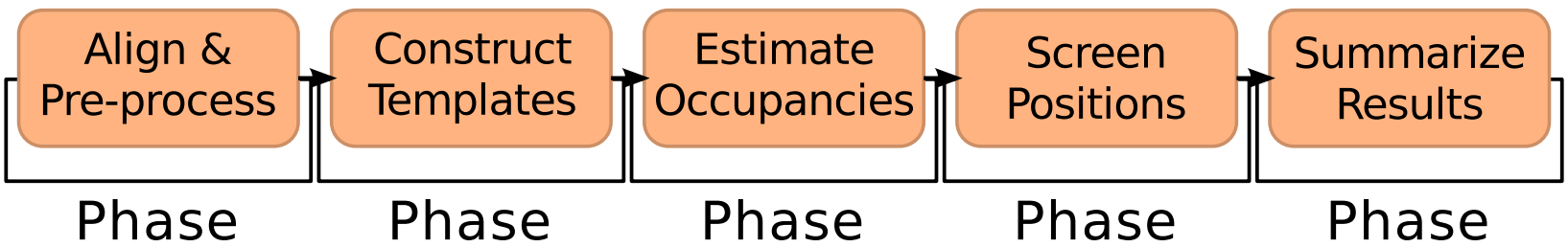
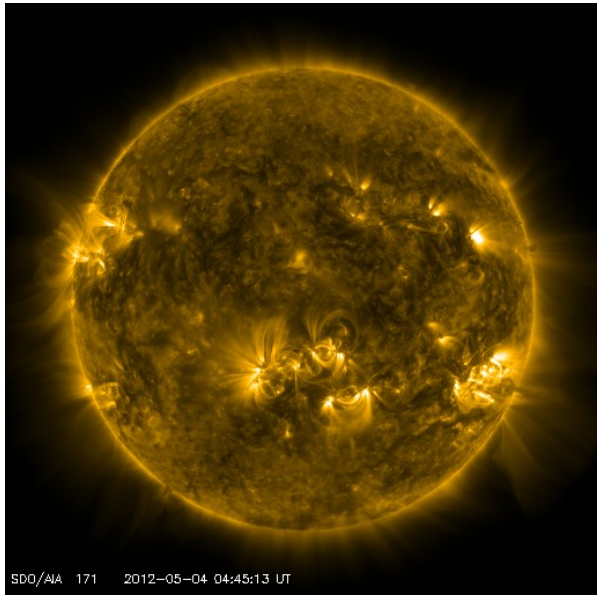


Massive solar data

- Preprocessing ubiquitous in massive-data astrophysics (Richards & Szalay)



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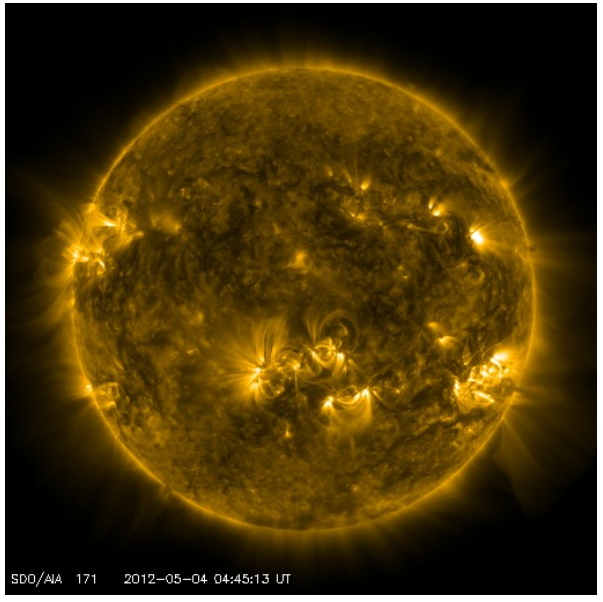

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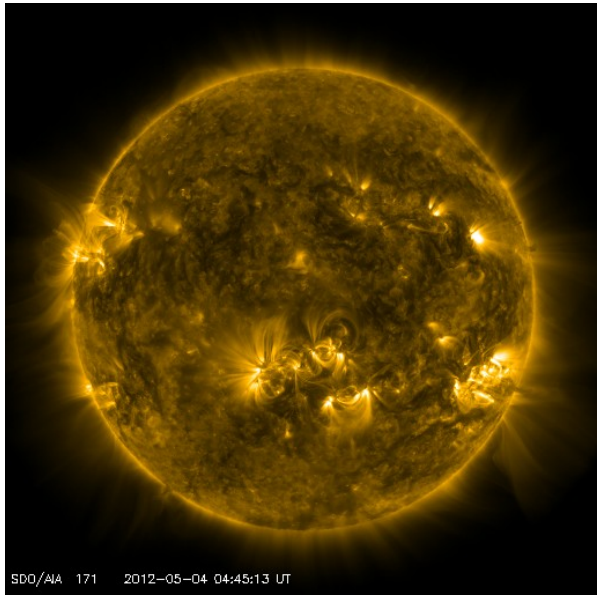

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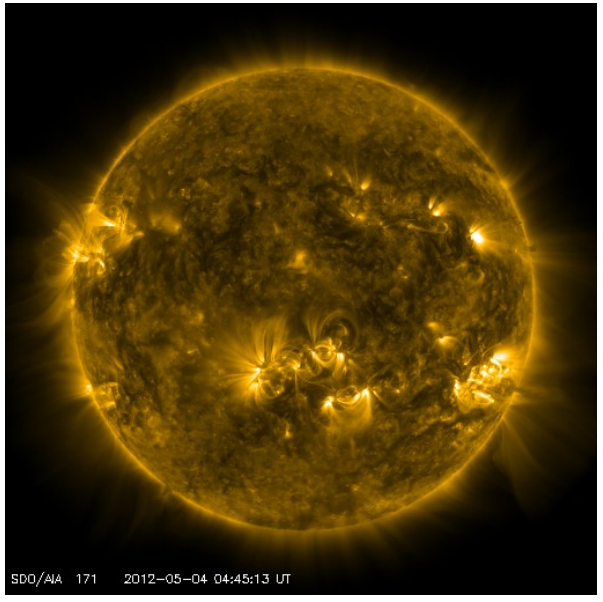

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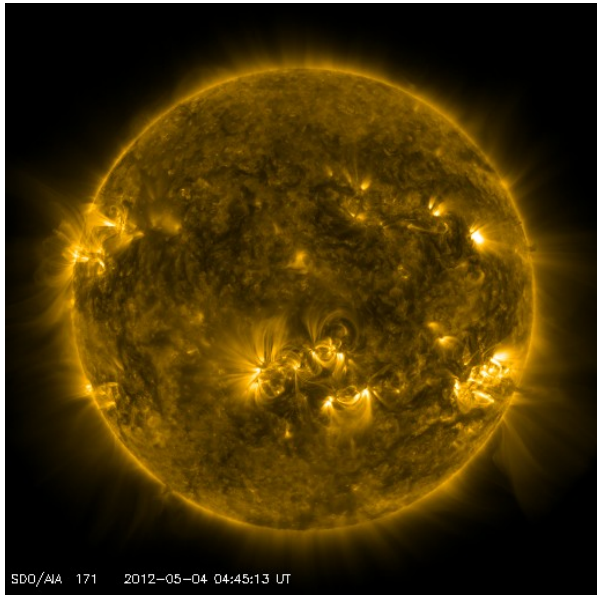
- Disputes in solar science community; cannot correct errors later on



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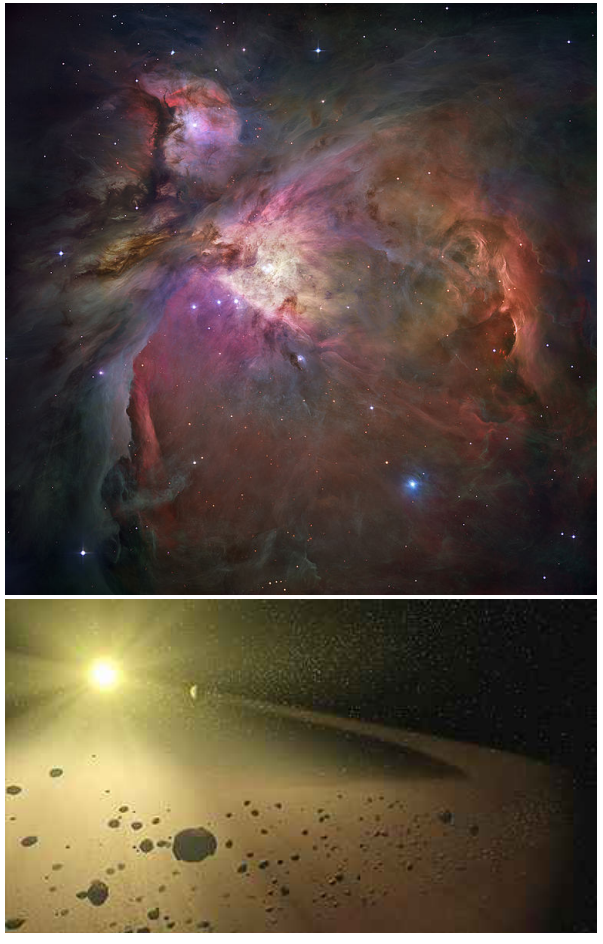
Indirect observations

- Dust clouds are centers of star formation



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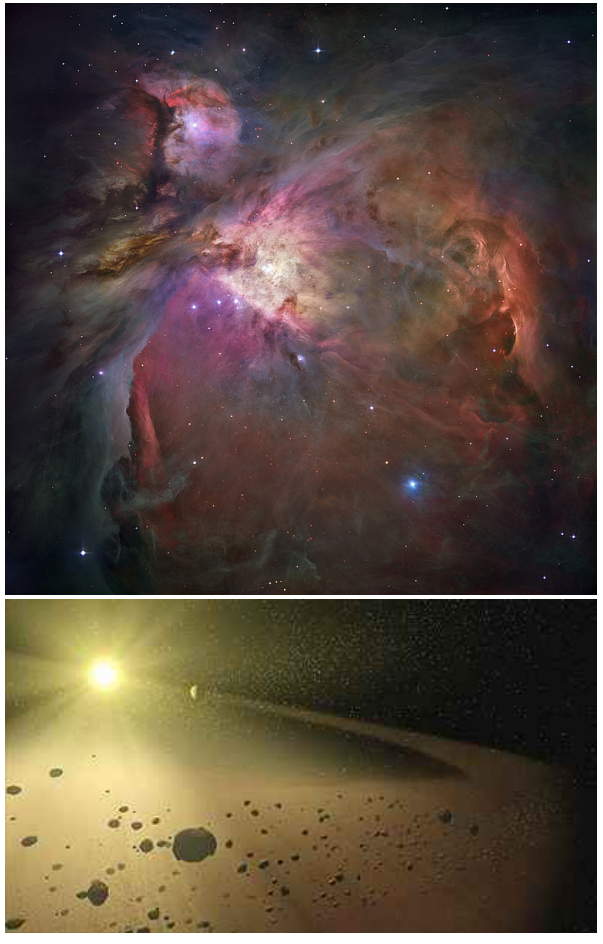

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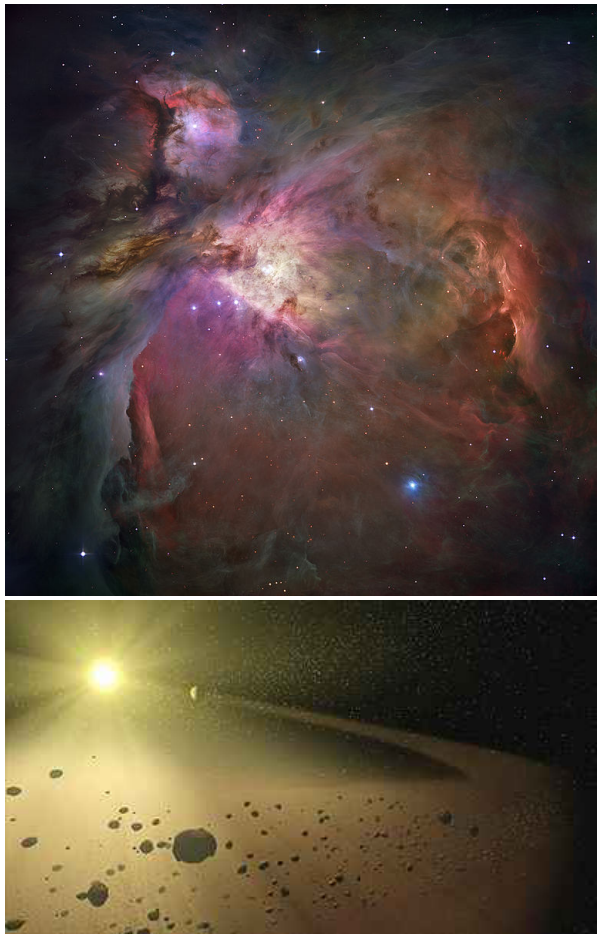

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Indirect observations

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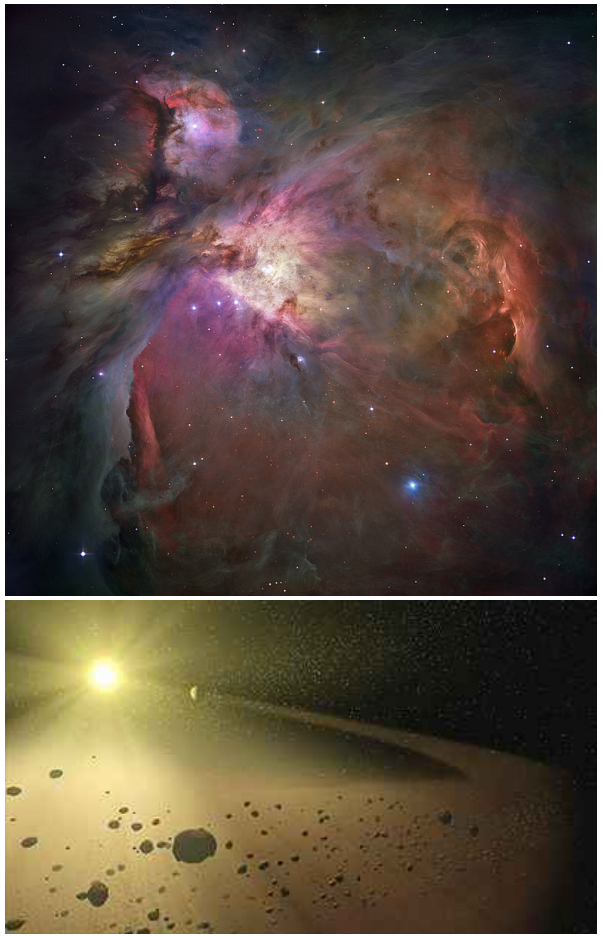
- Key relationship between temperature and dust density
- Must estimate these properties; cannot directly observe
- Incorrect preprocessing leads to backwards estimates of relationship (Kelly et al. 2012)



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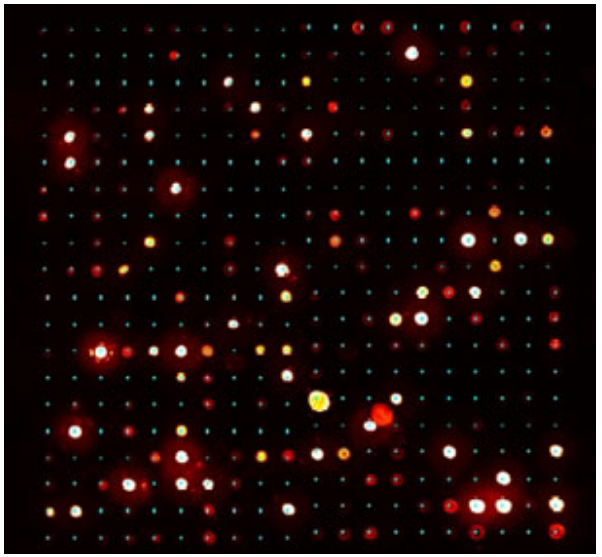
High-throughput biology

- Modern technologies measure thousands of genes or proteins at a time



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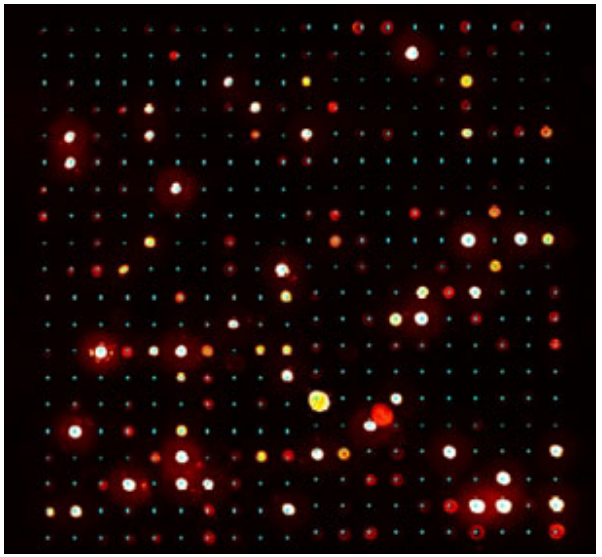

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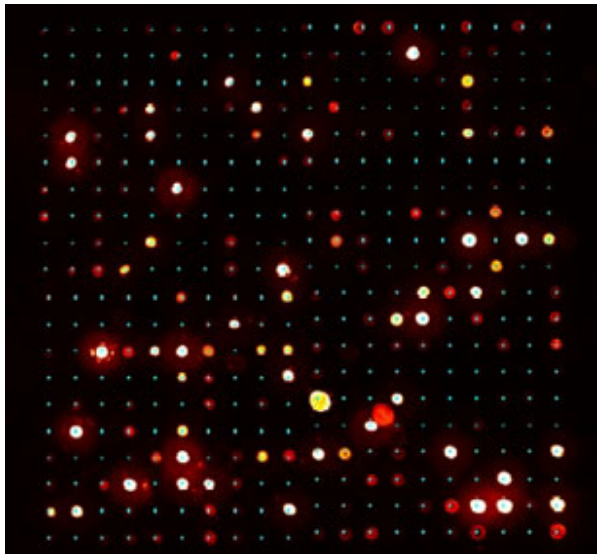

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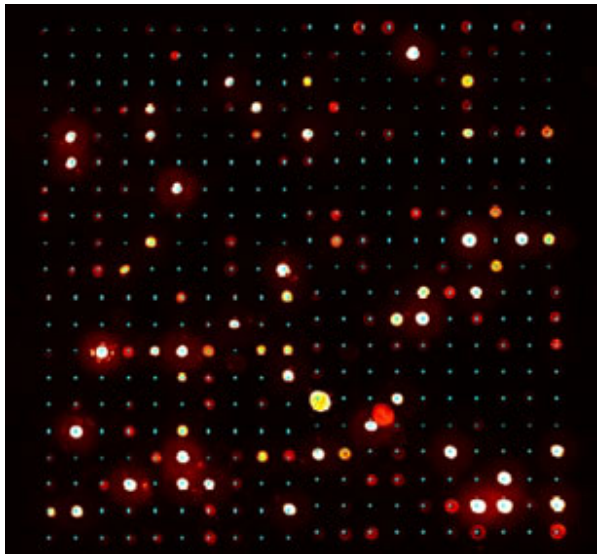
- Measure brightness of points on array; infer gene expression
- Sequencing brings its own, complex error processes



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Role of preprocessing — Microarrays

Standard methods based on heavily processed data

- Raw signals adjusted for background contamination
- Subsequent calibration for variation between arrays
- Then, statistical analysis of preprocessed results

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Why not a joint model?

- Computational scale
- Complexity of measurement process
- Separation of knowledge and effort is needed

Pitfalls and improvements

Missing pieces

- Measures of uncertainty not retained
- Irreversible calibration
- Processed results often insufficient for follow-up
- E.g.: Observe $Y = S + B$, correct for B, pass only point estimate of $\log S$. Problems?

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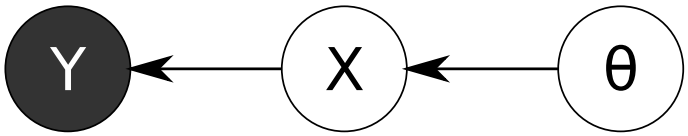
Remedies

- Wring rich summaries from observation models
- Retain summaries of uncertainty (e.g. Rick Steven's "graphs with probabilities" to replace alignments)
- Integrate richer information into downstream analyses

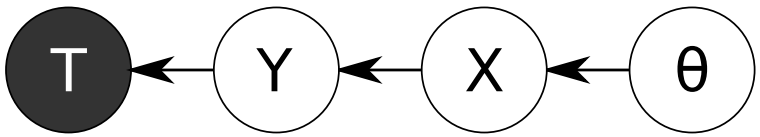
A model for two phases, in two phases

Building a framework to analyze and develop preprocessing techniques

Data-Generating Process



Downstream Analyst's Model



Notation

- $Y \in \mathbb{R}^N$ are observed data
- $X \in \mathbb{R}^J$ are scientific variables of interest
- θ are parameters governing scientific process
- T is the output from preprocessing

A model for two phases, phase two

Data-generating process — Preprocessor's model

$$p(Y, X|\theta) = p_Y(Y \mid X) \cdot p_X(X \mid \theta)$$

- Conditional independence structure
- Separation of knowledge
- X are missing data

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Downstream analyst's model

$$p(T, Y, X|\theta) = p_T(T|Y) \cdot p_Y(Y \mid X) \cdot p_X(X \mid \theta)$$

- Additional layer of processing
- X and Y are missing data

Revisiting examples

Indirect measurements in astrophysics

- Y are measurements from telescope, X are true features of dust cloud
- p_Y characterizes telescope's responses
- p_X and θ characterize structure of dust cloud

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Microarray measurement errors

- Y are measurements from array, X are true gene expressions
- p_Y characterizes measurement error
- p_X and θ characterize biological mechanisms

Defining multiphase procedures

Basic setup

- First phase provides $T = (\hat{X}, S)$
- Second phase has estimator $\hat{\theta}$ for each such T
- Different practical constraints induce different outputs

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Adaptation

- Second phase adapts; e.g., $T_0 = \hat{X}$ leads to simple mean, $T_1 = (\hat{X}, S)$ leads to weighted mean
- Extends to more than two constraints; e.g., aggregating data at multiple resolutions
- Need to regulate adaptation; for example, should do better with higher-resolution data

Regulating procedures

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- Models with principled estimation as generators of procedures

Role of constraints

Constraints are key

- Without tight constraints, dead ends and trivial results
- For example, optimal method simply computes optimal estimator with Y then passes it on
- Pragmatic constraints can yield deep theory (e.g. MI)

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Dual-use datasets

- If we could target $T(Y)$ to a single analysis, it's easy
- Practically, want preprocessed data for multiple uses
- Want $T(Y)$ both for inference on X and as input for further analyses
- Interpretability and modelability, not just efficiency

Two constraints for multiphase

Not too much more work

- Require complete-data estimator (using X) to be a version of multiphase estimator (e.g. nested models)
- For example, weighted least-squares regression when X would call for unweighted regression

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Spreading the load

- Require that first-phase procedures are distributable across researchers
- Build preprocessing on factored models for X

Factored models and sufficiency

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- Basic question: how can they determine what's needed to maintain sufficiency for θ?

Factored models and sufficiency

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- Suppose we want to distribute preprocessing across multiple researchers, each with their own experiments
- Assume particular model $p_X(X|\theta)$
- Basic question: how can they determine what's needed to maintain sufficiency for θ?
- Conversely, for which models p_X do we preserve sufficiency with given preprocessing?

Mathematical structure

- Assume observation model factors by researcher (i)

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- Constraining T_i to be sufficient for η_i

Mixture condition

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- Formally, when will sufficiency for η imply sufficiency for θ?
- Not enough for working model to be (marginally) correct for each Y_i
- Sufficient condition: mixture

$$p_X(X|\theta) = \int_{\mathrm{H}} \prod_i p_W(X_i|\eta_i) \, \mathrm{d}P(\eta|\theta)$$

Implications and extensions

Applied guidance

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- Must look to models that include yours hierarchically
- However, can obtain results without sufficiency for X

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Theoretical loose-ends

- Mixture condition not necessary
- Counterexamples to necessity based on unparameterized dependence

Classical results

Doing the best with what you get

- For fixed preprocessing, what bounds performance?
- In large samples, fraction of missing information ($F = I_Y^{-1} I_{Y|T}$) determines lower bound on variance
- Formally, relative excess variance converges to F: $\text{Var}(\hat{\theta}(T))^{-1} \text{Var}(\hat{\theta}(T) - \hat{\theta}(Y)) \to F$

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Giving all that you can

- What is good preprocessing with $\hat{\theta}(T)$ fixed?
- All* admissible $T(Y)$ are (generalized) Bayes rules
- Extension of standard complete-class results
- Further bounds from multiple imputation (MI) theory

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- Defined model and multiphase procedures
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Theoretical cornerstones

- Condition for distributed preprocessing
- Performance bounds for multiphase settings

Coming attractions

Theory

- Evaluation of preprocessing methods for design and analysis
- Constrained optimality results for broadly-applicable multiphase strategies

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Applications

- Improved multiphase methods for biological and astronomical problems
- Multiphase-based computational strategies for massive data

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- Xiao-Li Meng
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