

# Rapid Biomedical Knowledge Base Construction from Unstructured Data

## Snorkel Workshop

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# Day 1: Agenda Outline

## Designing Labeling Functions (LFs)

- Pattern Matching & Distant Supervision
- Evaluating LF Performance
- Snorkel API / Writing Labeling Functions

## Generative Model: Unifying Supervision

- Simple Baseline: Majority Vote
- Automatically Learning LF Accuracies
- LF Dependency Learning

## Discriminative Model: “Compiling” Rules into Features

- Training with Probabilistic Labels
- The Death of Manual Feature Engineering
- Why Do We Need the Discriminative Model?



# Day 1: Agenda Outline

## **Application Development:**

### **Introducing Schemas and Evaluation Plans**

- Day 2 Preview: Designing a Good Evaluation Plan
- Schema Design Template

## **Welcome Reception**



# Terminology

## Entity

Concepts that can be separated into meaningful categories



## Relation

Semantic associations between 2 or more entities



## Knowledge Base

A repository for structured information

A network of all **chemical-induced disease relations** found in **PubMed**

# Imagine for a moment ...



Entertainment News Website

The entertainment news website TMZ wants **YOU** to build a state-of-the art text-mining system for tracking celebrity marriage gossip...

Being a top-notch (somewhat mercenary) data scientist...

You quickly recognize this as a **relation extraction task**

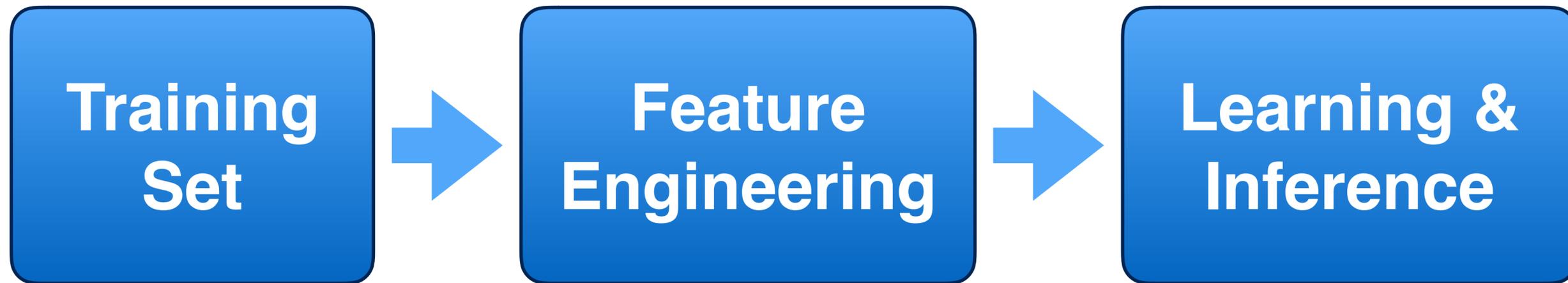
# Extract Spouse Mentions from Text

**TASK:** Build a **knowledge base** of married couples by extracting mentions of **spouses** from news articles

Jeffrey Navin, 56, and his wife, Jeanette, 55, a school paraprofessional on Facebook by Rachel Hattingh and her husband Graham Marshall, a Brecht-Schall was married to actor Ekkehard Schall, a stalwart of

Sentences containing mentions of married couples

# Traditional Machine Learning Approach...

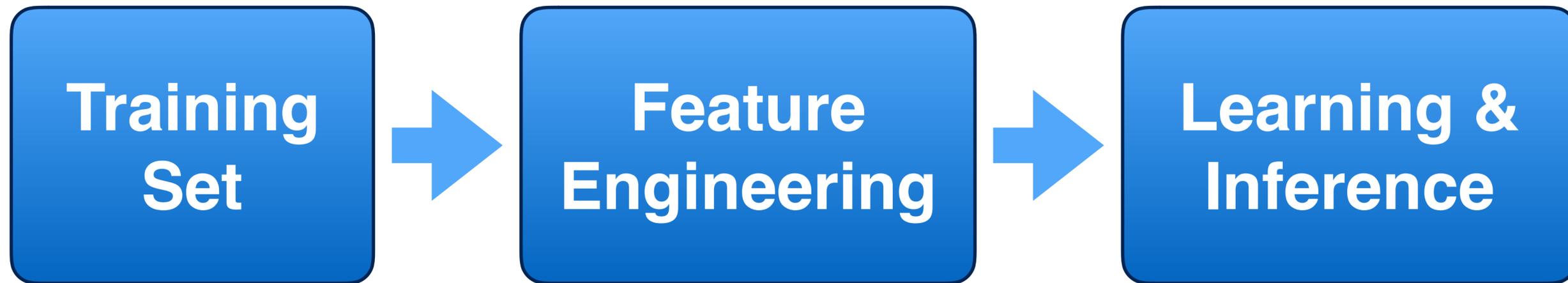


Manually  
Label Data

Manually  
Define Features

Train a Model

# Traditional Machine Learning Approach...



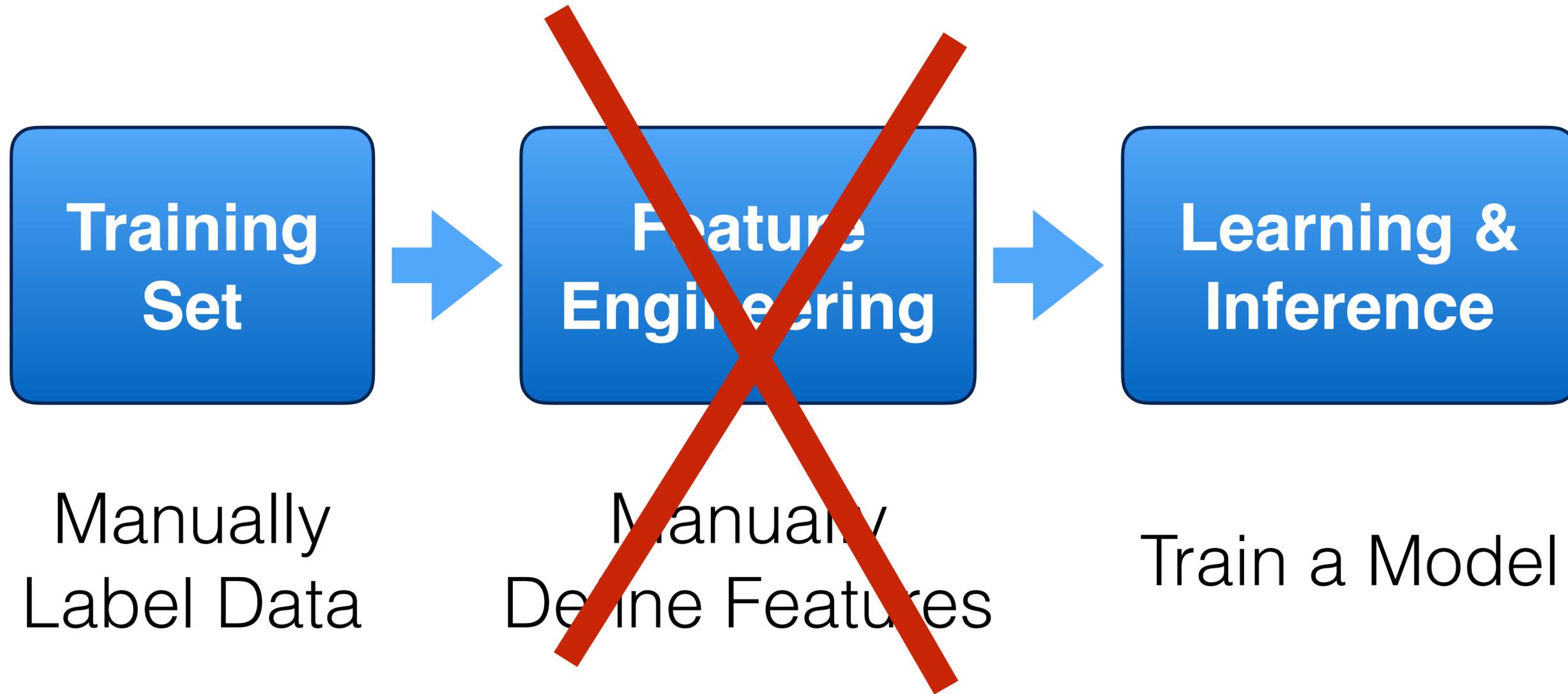
Manually  
Label Data

Manually  
Define Features

Train a Model

**Requires non-trivial engineering effort!**

# Traditional Machine Learning Approach...



**Deep Learning Killed  
Feature Engineering**

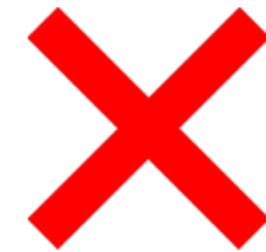
# Traditional Machine Learning Approach...

but we still need to label a bunch of data!

Ellen DeGeneres and wife Portia De Rossi have seemingly shut down divorce rumors with a joint outing in Los Angeles.



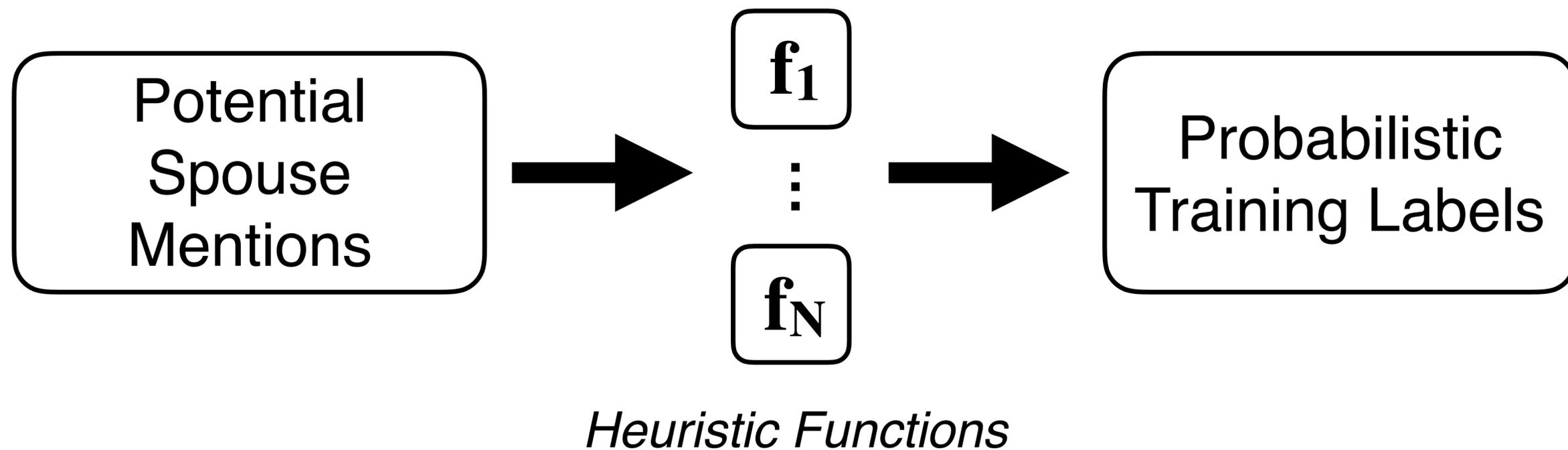
Khloe Kardashian says she's DEFINITELY down to marry Tristan Thompson ... even though he hasn't exactly proposed yet.



Repeat hundreds or thousands of times...

# Snorkel / Data Programming Approach...

Write *heuristics* to noisily label data!



**Programmatically generate training data**



# Labeling Functions: Intuition and Overview

# Labeling Functions

Side-by-Side was started on Facebook by **Rachel Hattingh** and her husband **Graham Marshall**, a London homeless charity chief executive, from Stanford-le-Hope.

Is this a true spouse mention?  
What evidence informs your decision?

# Labeling Functions

Former U.S. president **Barack Obama** and first lady **Michelle Obama** arrive to talk about the Obama Presidential Center during a community event at the South Shore Cultural Center on May 3 in Chicago, Illinois.

Is this a true spouse mention?  
What evidence informs your decision?

# Labeling Functions

Human annotators leverage  
**real-world knowledge, context,**  
and **common-sense heuristics**  
to make labeling decisions

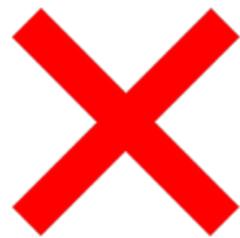
We can model parts of this process by  
encoding these rules as functions ...

# Labeling Functions

## Labeling Functions (LFs)

Black box functions that label subsets of data

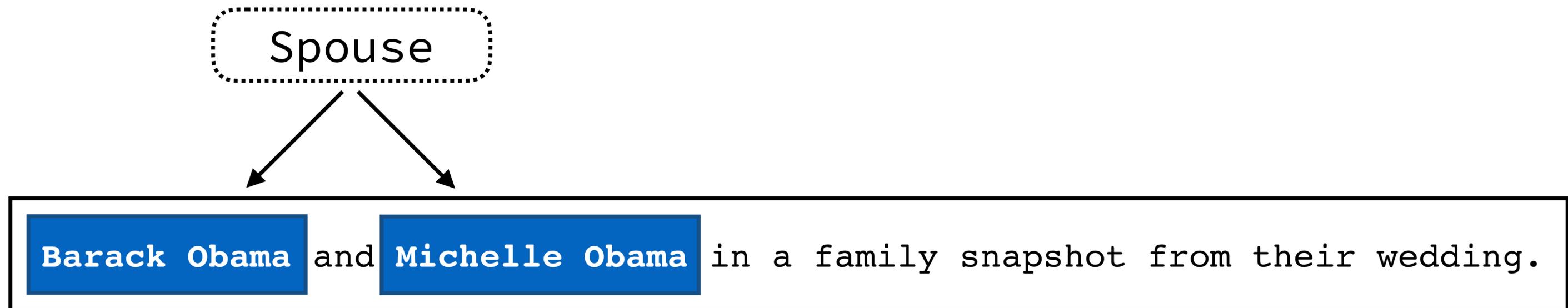
$\{-1, 0, 1\}$



`{Negative, Abstain, Positive}`

# Candidates

All pairs of **people's names** in a sentence



# Labeling Functions

**Candidates** includes **true** and **false** instances

**SENT\_ID 1:** Jeffrey Navin, 56, and his wife, Jeanette, 55, a scho

**SENT\_ID 2:** Khloe Kardashian says she's DEFINITELY down to marry

(Jeffrey Navin, Jeanette)



(Khloe Kardashian, Tristan Thompson)



# Labeling Functions

**Goal:** Provide (potentially weak) correlated signal with true class labels

Apply labeling functions to all candidates

Predict both **positive** and **negative** labels

# Labeling Functions



## INSIGHT

People with the same last name *might* be married

... photos taken of President **Barack Obama**  
and first lady **Michelle Obama** during ...



## INSIGHT

If '**boyfriend**' or '**girlfriend**' appear between people mentions, the pair are probably *not* married

... **Pippa** is engaged to her hedge fund  
manager **boyfriend James Matthews** ...

# Labeling Functions

## Implement these rules as Python functions



```
def LF_same_last_name(c):  
    """  
    Label as positive if both  
    """  
    p1_last_name = last_name(c.person1.get_span())  
    p2_last_name = last_name(c.person2.get_span())  
    if p1_last_name and p2_last_name and p1_last_name == p2_last_name:  
        if c.person1.get_span() != c.person2.get_span():  
            return 1  
    return 0
```



```
def LF_dating(c):  
    dating = {'boyfriend', 'girlfriend'}  
    return -1 if len(dating.intersection(get_between_tokens(c))) > 0 else 0
```

# Labeling Functions

Labeling functions can be **noisy**

People with the same last name *might* be married

TRUE

PREDICTED



... photos taken of President **Barack Obama** and first lady **Michelle Obama** during ...



**Mary-Kate Olsen** and **Ashley Olsen** (born June 13, 1986), also known as the Olsen twins collectively...



**Tom Hanks** reveals his 28-year marriage to **Rita Wilson** almost never happened.



# Labeling Functions: Design Strategies

# Labeling Functions

Jeffrey Navin, 56, and his wife, Jeanette, 55, a school parapr  
book by Rachel Hattingh and her husband Graham Marshall, a London h  
Ellen DeGeneres and wife Portia De Rossi have seemingly

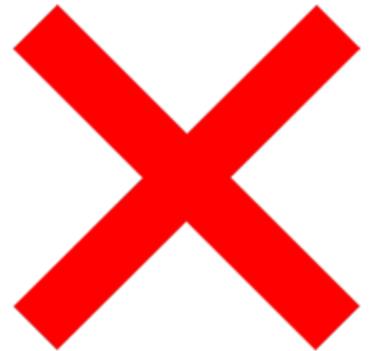
Previously, we used common-sense **patterns** or **keywords** to label a person pair as married or not

# Labeling Functions

Jeffrey Navin, 56, and his wife, Jeanette, 55, a school parapr  
book by Rachel Hattingh and her husband Graham Marshall, a London h  
Ellen DeGeneres and wife Portia De Rossi have seemingly

## Pattern-based Labeling Functions

# Labeling Functions



## INSIGHT

If 'boyfriend' or 'girlfriend' appear between people mentions, the pair are probably *not* married

... **Pippa** is engaged to her hedge fund manager **boyfriend James Matthews** ...

These are implemented using **string matching** via **regular expressions** and other heuristics

# Labeling Functions

We can also use other sources of information to generate LFs

## **Distant Supervision Labeling Functions**

These use an existing database of known facts to generate noisy labels

# Labeling Functions: Distant Supervision

```
def known_spouse(x):  
    pair = (x.person1_id, x.person2_id)  
    return 1 if pair in KB else 0
```

Former U.S. president **Barack Obama** and  
first lady **Michelle Obama** arrive to talk ...



**Knowledge Base (KB)**

CONTAINS

(**A** **B**)



**Label = True**

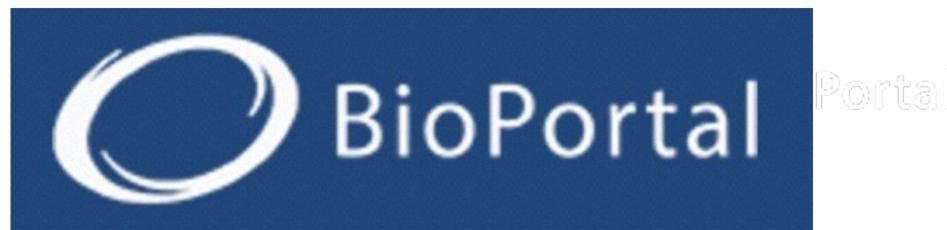
# Labeling Functions: **Distant Supervision**



orphanet



**UMLS**  
Unified Medical  
Language System



Many **public knowledge bases**  
are available, especially in **biomedicine**

# Labeling Functions: **Distant Supervision**



Public semantic **knowledge base**, let's use this resource for distant supervision

<http://wiki.dbpedia.org/>



# Labeling Functions: Scoring Metrics

# Labeling Function: Metrics

How do we assess the quality of our labeling functions?

# Labeling Function: Metrics

**Accuracy:** The percentage of candidates a labeling function labels correctly

**Coverage:** The percentage of all candidates that are labeled by  $\geq 1$  LFs

**Conflict:** The percentage of candidates with  $> 1$  labels that disagree

# Labeling Function: Metrics

**Assessing empirical accuracy  
requires some **ground truth labels****

**Dev Set:** A small set (~100 candidates)  
of human labeled examples we can use  
to guide LF development

# Labeling Function: Metrics

Ideally, we want **high-coverage, high-accuracy** LFs

LFs need to label with **probability better than random chance**

**Conflict is actually good** — it allows our algorithm to learn information about the LF

# Terminology

$$\text{Precision} = \frac{tp}{tp + fp}$$

How often a predicted label is correct

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$$\text{Recall} = \frac{tp}{tp + fn}$$

Given the known total number of positive instances, how many were labeled correctly

---

$$F_1\text{-score} = \frac{\textit{precision} * \textit{recall}}{\textit{precision} + \textit{recall}}$$

Harmonic mean of precision and recall



# Snorkel API (Hands-on Exercises)

# Snorkel API

## Open Tutorial Notebook

Workshop\_1\_Snorkel\_API.ipynb

- Introduce Jupyter notebooks
- Fill out your email/username
- Introduce Candidate classes
- Complete exercises 1 & 2



# Writing Labeling Functions (Hands-on Exercises)

**TIME: 60 Minutes**

# Writing Labeling Functions

## Open Tutorial Notebook

`Workshop_2_Writing_Labeling_Functions.ipynb`

- Introduce labeling function factories
- Complete tutorial examples



# Generative Model: Unifying Supervision

# Terminology

## Generative Model

$$P(x,y)$$

Learn the joint distribution of  $(x,y)$

### Example Classifiers

Naive Bayes

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## Discriminative Model

$$P(y|x)$$

Learn the conditional probability of  $y$  given  $x$

### Example Classifiers

Support Vector Machine (SVM)

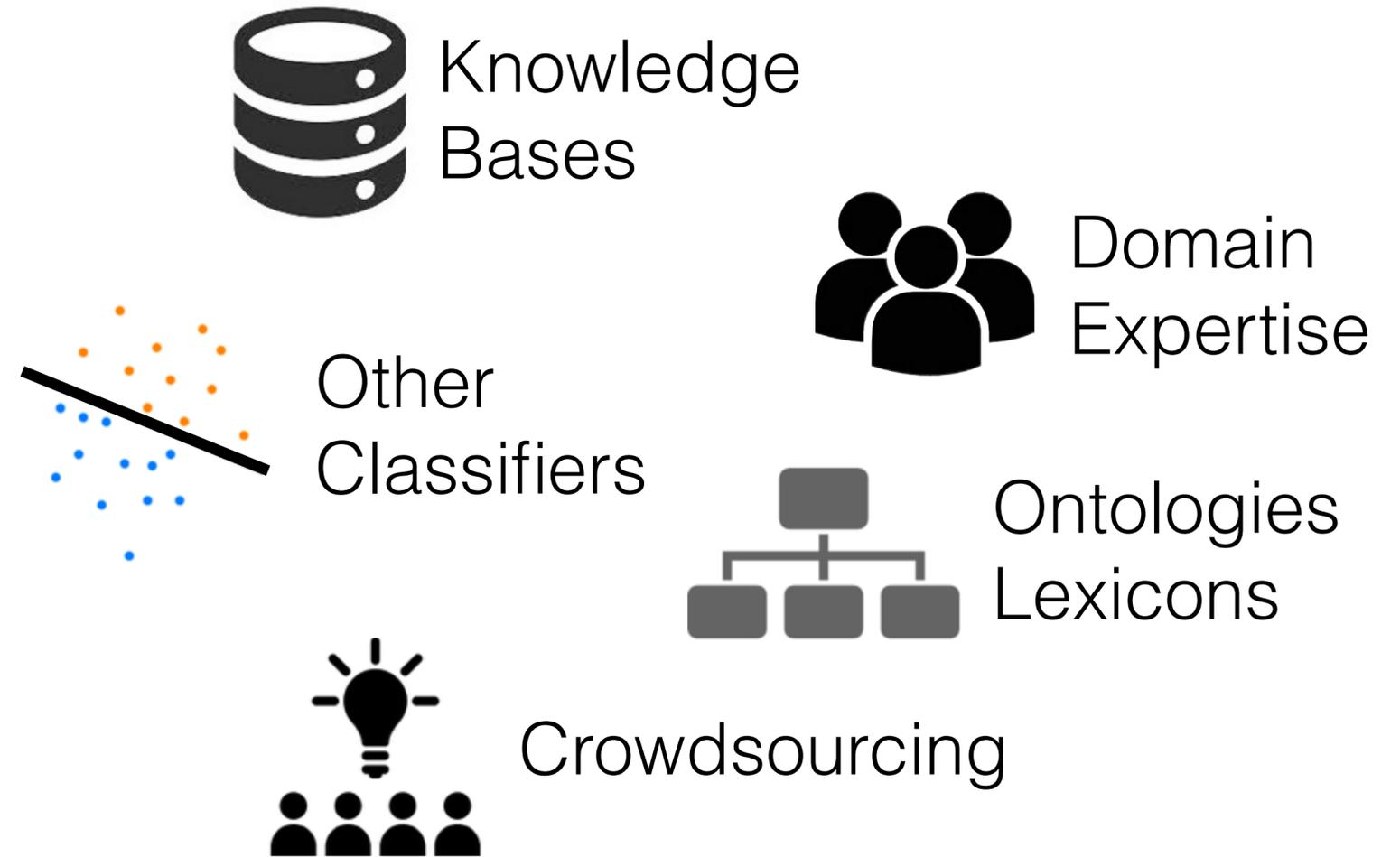
Logistic Regression

Deep Neural Networks (LSTMs)

# Generative Model: Unifying Weak Supervision

Labeling functions allow for **radically weaker labels**

These labels can be noisy, conflicting, and come from a **variety of inputs**



**Key Idea:** Labeling functions encode all these forms

# Intuition: How Does it Work?

Simplest way to unify LFs is  
**unweighted majority vote**



# Intuition: How Does it Work?

As long as most people vote correctly ( $p > 0.5$ ), adding more people improves the accuracy of majority vote\*

\* Condorcet's Jury Theorem

A black and white silhouette illustration of a crowd of people. Many individuals have their arms raised, with some hands open and others in various gestures, suggesting a lively event or a voting process. The silhouettes are layered, with some in the foreground and others receding into the background, creating a sense of depth and a large group of people.

# Intuition: How Does it Work?

LFs have different **latent accuracies**  
Unweighted majority vote ignores this!

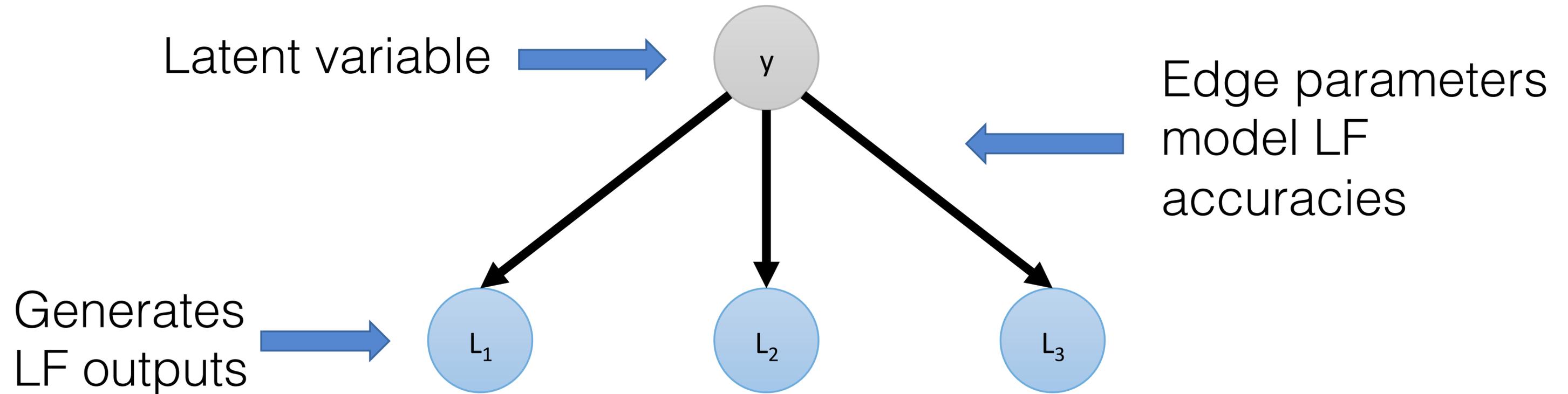


# Intuition: How Does it Work?

We want to learn these latent accuracies  
**without labeled data** by leveraging  
**overlap** and **conflict** of LFs

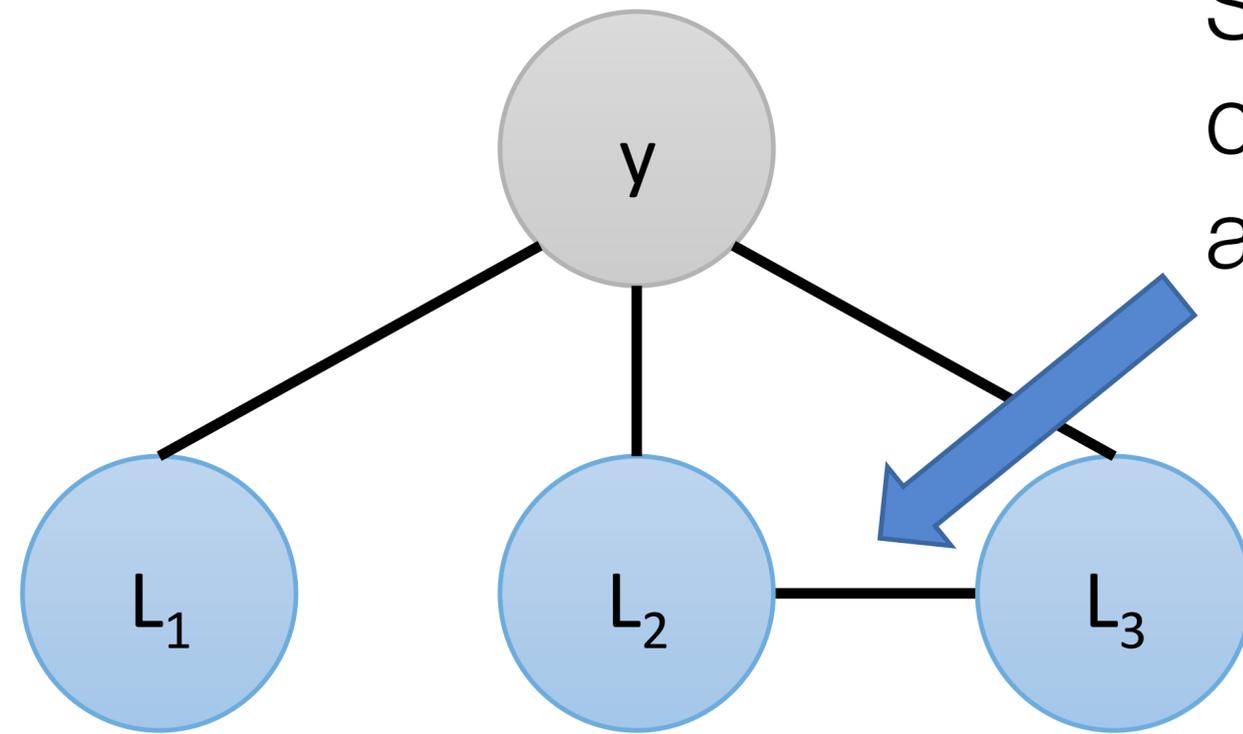


# Generative Model: Unifying Weak Sources ...



We maximize the marginal likelihood of the LFs to learn parameters  
Intuitively, compares their agreements and disagreements

# Generative Model: Structure Learning



Snorkel can automatically detect correlations and other dependencies among LFs to correct their accuracies

Adds, on average, a **1.5 F1 boost** to models — for free

[Bach et al., ICML 2017]

**See the Snorkel blog post for more details**

[https://hazyresearch.github.io/snorkel/blog/structure\\_learning.html](https://hazyresearch.github.io/snorkel/blog/structure_learning.html)

# Structure Learning

Data programming assumes LFs make **independent labeling decisions**



If LFs make **correlated decisions**, independent of the true label, the MLE of the parameters will **overweight LFs latent accuracies**

# Structure Learning

## When does this happen?

- Using **multiple, overlapping ontologies** for distant supervision
- LFs only differ due to **tunable parameters**, like context window size.
- Many more!



# Training the Generative Model (Hands-on Exercises)

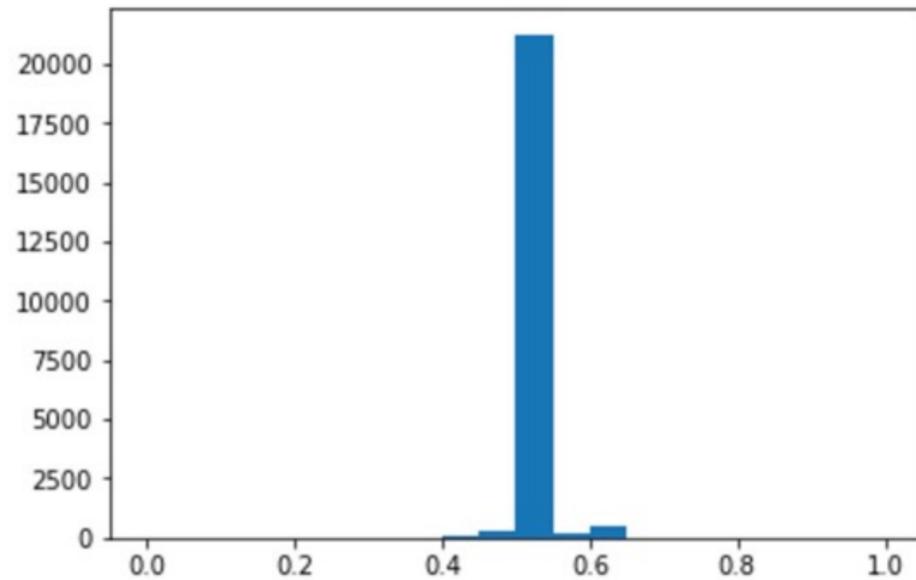
# Training Generative Models

## Open Tutorial Notebook

`Workshop_3_Generative_Model_Training.ipynb`

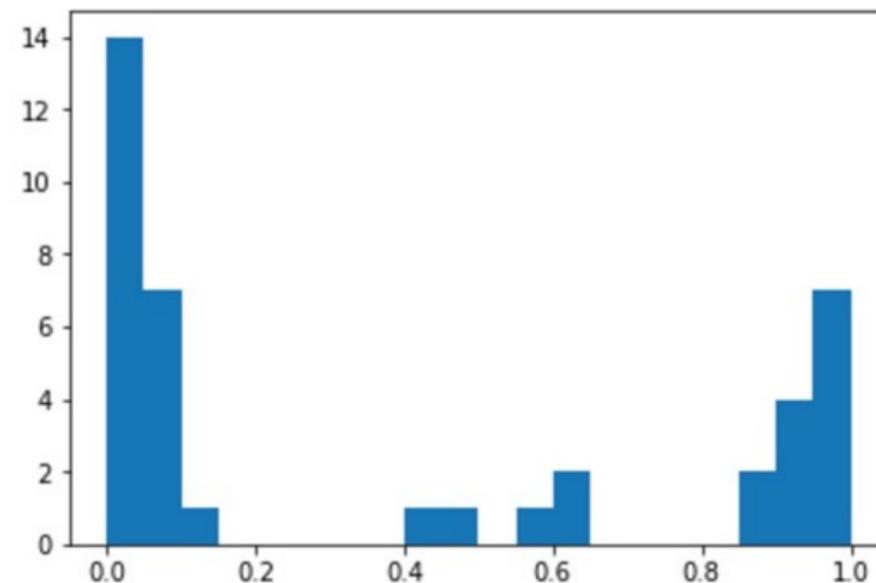
- Majority vote
- Training the generative model
- Interpreting Marginals
- Learning dependencies

# Generative Model: Interpreting Marginal Distributions



This is probably the first set of marginals you'll generate. These are **BAD!**

Everything's clustered at 0.5, i.e, **no labels**



This are the marginals you want!. These are **GOOD.**

Clear differentiation between 0.0 / 1.0



# Refine Writing Labeling Functions (Hands-on Exercises)

**TIME: 45 Minutes**



# **Discriminative Model: “Compiling” Rules into Features**

# Snorkel API

**Open Tutorial Notebook**

`Workshop_4_Discriminative_Model_Training.ipynb`

- Train an LSTM model

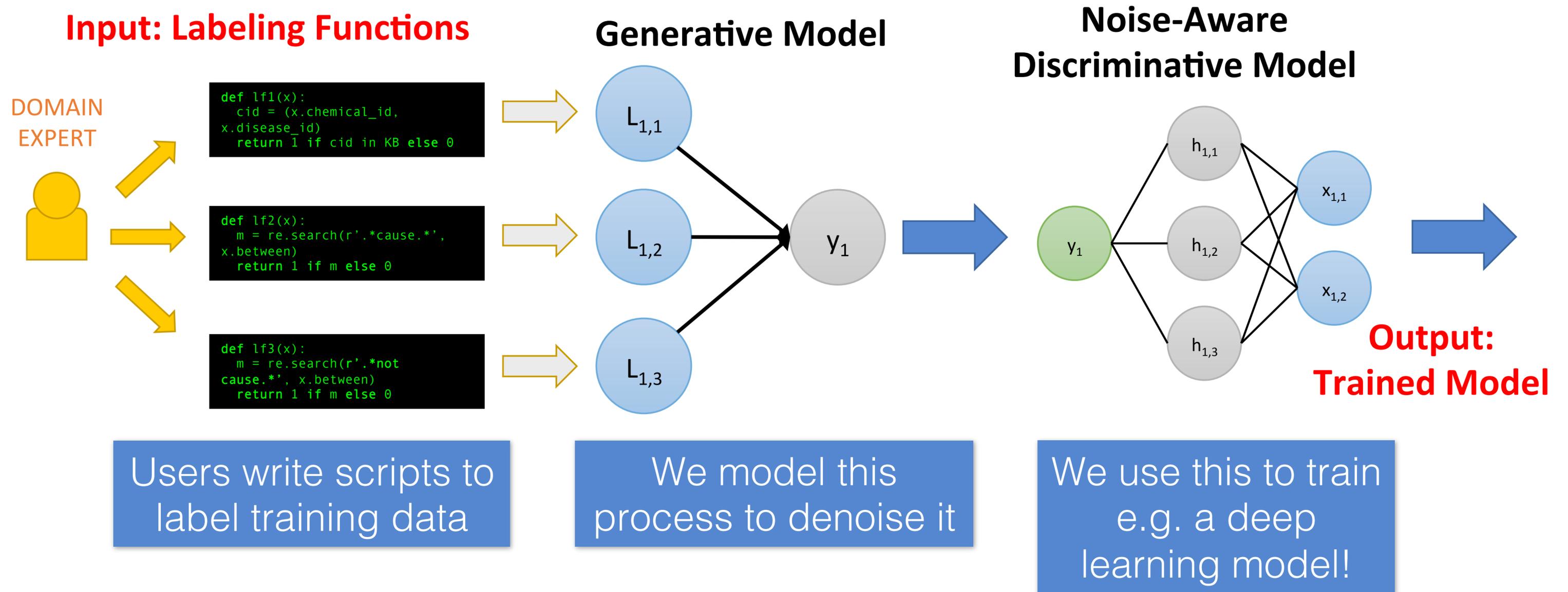
**This takes ~10 minutes. Start now!!**

# Discriminative Model

The output of the generative model is a set of **probabilistic training labels**

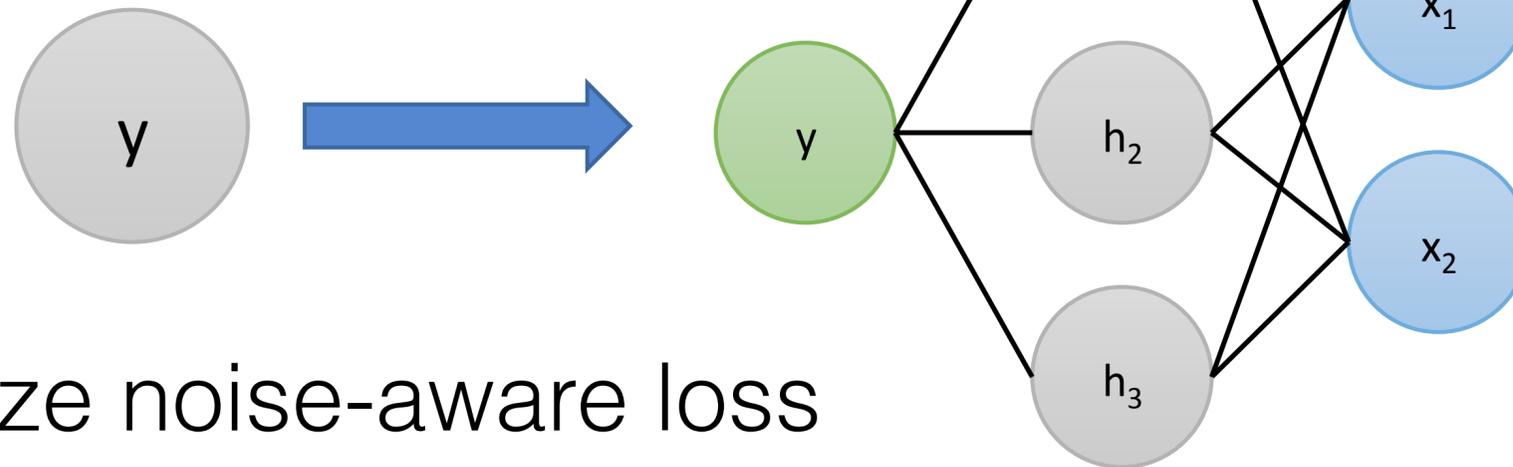
We now want to use these labels to train our final discriminative model

# Discriminative Model: Full Snorkel Pipeline



# Discriminative Model

Train on marginals from generative model



Minimize noise-aware loss

Generalization error decreases at same asymptotic rate as in supervised setting, except **in amount of unlabeled data**

[Ratner et al., NIPS 2016]

# Training a *Noise-aware* Discriminative Model

## Supervised Learning Loss Function

$$\hat{w} = \operatorname{argm} \operatorname{in}_w \frac{1}{N} \sum_{i=1}^N l(w, x^{(i)}, y^{(i)})$$

## Noise-aware loss

$$\hat{w} = \operatorname{argm} \operatorname{in}_w \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{(y, \Lambda) \sim \pi} [l(w, x^{(i)}, y^{(i)} = y)]$$

Simple change for Logistic Regression, SVMs, LSTM (neural networks)

# Discriminative Model

Why can't we just use the generative model for our final predictions?

The discriminative model learns a **feature representation** of our **LFs**

This makes it better able to generalize to unseen candidates

# Discriminative Model

As a result, we see much better recall!

	<b>Precision</b>	<b>Recall</b>	<b>F1</b>
Majority Vote	76.4	67.3	71.5
Generative Model	67.4	<b>77.9</b>	72.3
CRF	<b>81.5</b>	75.8	78.5
BiLSTM-CRF	80.7	77.6	<b>79.1</b>

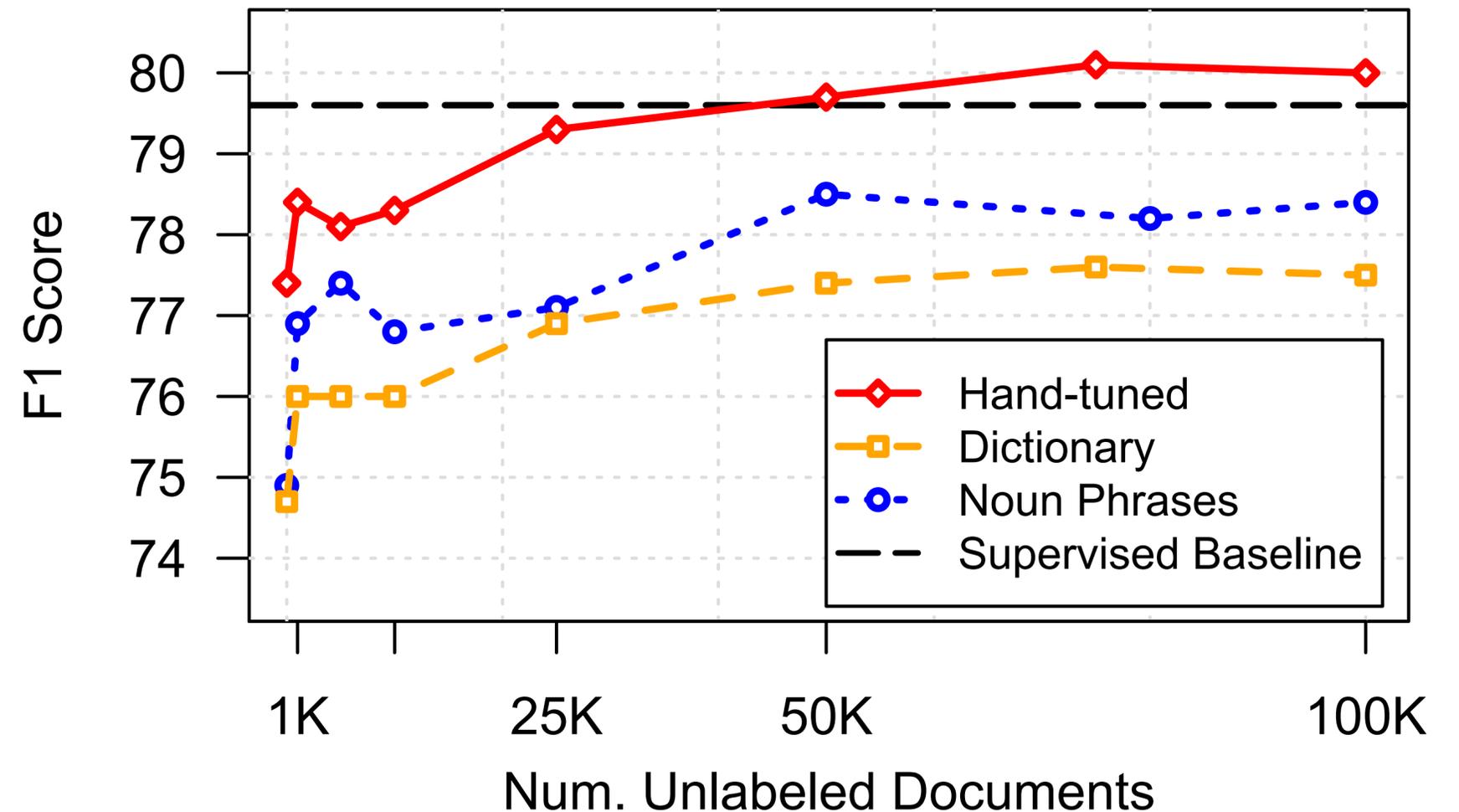
— CDR disease name tagging

[Fries et al., 2017]

# Discriminative Model

We can now **automatically generate large-scale training sets**

We can **match or exceed** supervised learning performance



Tagging disease names in PubMed

[Fries et al., 2017]



## Refine Writing Labeling Functions (Hands-on Exercises)

**TIME: 45 Minutes**



# **Application Development: Introducing Schemas and Evaluation Plans**

# Application Design

*Two critical questions for any new application*

What **information** am I **extracting**?

Once extracted, what is the **utility**  
of this **new information**?

# Application Design: Project Template

*We've provided a project template for tomorrow's discussion*

1. Motivation
2. Task Overview
3. Data Set Overview
- 4. Schema Design**
5. Validating Your Extraction Models
6. External Utility

# Application Design: Schema

**Schema:** The formal definition of what we are extracting from text. This is the structured representation of our facts.

Spouse ( PERSON, PERSON )

Chemical-induced Disease (CHEMICAL, DISEASE)

Side Effect ( DRUG, SYMPTOM/SIGN )

**Formally defining these entities and relations is the most important step in building a Snorkel application!**

# Contact Us



## Code Issues?

GitHub: Snorkel Issues

<http://snorkel.stanford.edu>

<https://github.com/HazyResearch/snorkel>

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