

Introduction to Machine Learning and Probabilistic Modeling

Piyush Rai

Probabilistic Machine Learning (CS772A)

Dec 30, 2015

Course Logistics

- **Course website:** http://www.cse.iitk.ac.in/users/piyush/courses/pml_winter16/PML.html
- **Instructor:** Piyush Rai (<http://www.cse.iitk.ac.in/users/piyush/>)
- **TAs:** Milan Someswar, Vinit Tiwari, Rahul Kumar Patidar
- **Discussion site:**
<https://piazza.com/iitk.ac.in/secondsemester2016/cs772a/>
- **Background assumed:** basics of linear algebra, multivariate calculus, **probability and statistics**, optimization, programming (MATLAB, R, Python).

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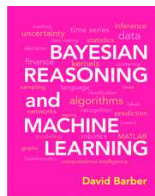
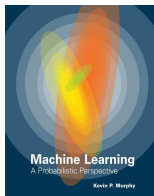
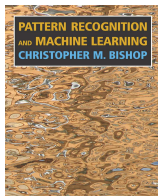
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 - Project: 30% (to be done in groups of 3 students)

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 - Project: 30% (to be done in groups of 3 students)
 - **Note:** A really awesome project (e.g., publishable piece of work) may help you automatically get an A grade. You may propose your own project or talk to me for ideas. The project has to be (at least loosely) related to probabilistic ML. More details coming soon.

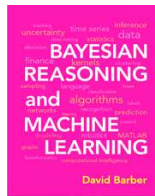
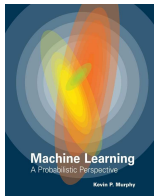
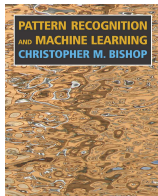
Books

Some books with a bent towards *probabilistic* machine learning:

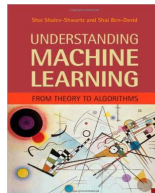
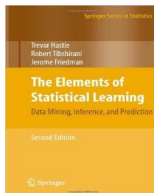
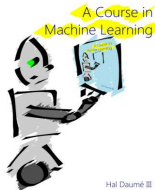


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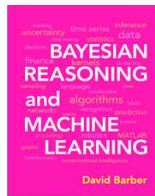
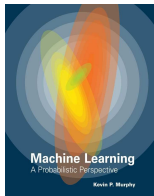
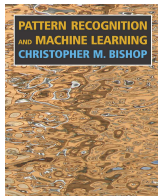


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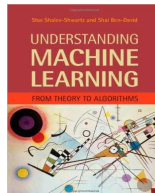
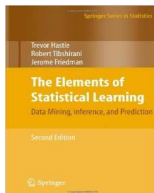
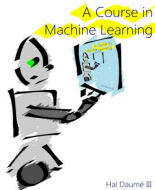


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Some other books on machine learning:



Not shown: many excellent books on special topics (kernel methods, online learning, Bayesian learning, deep learning, etc.). Ask me if you want to know.

Intro to Machine Learning

Machine Learning

- Creating programs that can automatically **learn rules** from data
“Field of study that gives computers the ability to learn without being explicitly programmed” (Arthur Samuel, 1959)

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- Traditional way: Write programs using hard-coded (fixed) rules

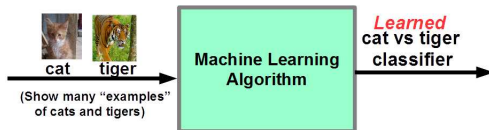


Machine Learning

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- Machine Learning (ML): **Learn rules** by looking at the data

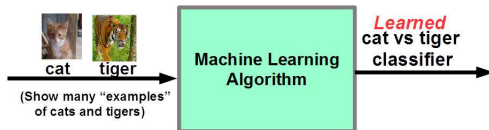


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- Machine Learning (ML): **Learn rules** by looking at the data



- Learned rules must generalize (do well) on future "test" data (idea of **generalization**; more on this later)

Machine Learning in the real-world

Broadly applicable in many domains (e.g., finance, robotics, bioinformatics, computer vision, NLP, databases, systems, etc.). [Some applications:](#)

- Information retrieval (text, visual, and multimedia searches)
- Machine Translation
- Question Answering
- Social networks
- Recommender systems (Amazon, Netflix, etc.)
- Speech/handwriting/object recognition
- Ad placement on websites
- Credit-card fraud detection
- Weather prediction
- Autonomous vehicles (self-driving cars)
- Healthcare and life-sciences
- .. and many more applications in sciences and engineering

Data and *Data Representation*..

Data Representation

- ML algorithms work with data represented as a set of features/attributes
- One popular representation: **bag-of-features**

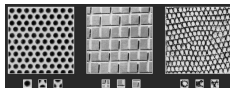


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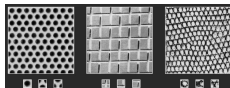


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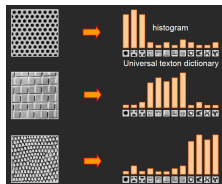
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- Now represent each example using the frequency of each feature



Data Representation

Another example: representing text data. Consider the following sentences:

- John likes to watch movies
- Mary likes movies too
- John also likes football

The feature vocabulary consists of 8 unique words

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Here is the **bag-of-words** feature representation of these 3 sentences

	John	likes	to	watch	movies	Mary	too	also	football
Sentence 1	1	1	1	1	1	0	0	0	0
Sentence 2	0	1	0	0	1	1	1	0	0
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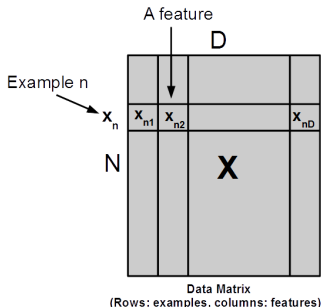
Note: Not necessarily the most optimal/most expressive feature representation

Feature representation learning is a very active area of research in ML (there is even a dedicated conference on this topic: ICLR)

Data Representation

We will (usually) assume that:

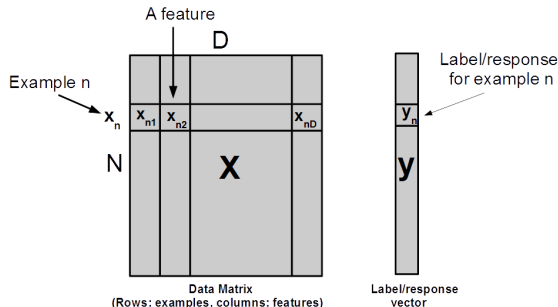
- \mathbf{X} denotes data in form of an $N \times D$ feature matrix
- N examples, D features to represent each example
- Each row is an example, each column is a feature
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- \mathbf{y} denotes labels/responses in form of an $N \times 1$ label/response vector
- y_n denotes label/response of the n -th example \mathbf{x}_n

Types of Machine Learning problems..

Supervised Learning

Supervised Learning

- Given: Training data as **labeled examples** $\{(x_1, y_1), \dots, (x_N, y_N)\}$
- Goal: Learn a rule (“function” $f : x \rightarrow y$) to predict **outputs** y from **inputs** x

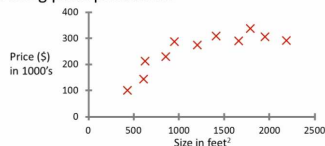
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 - **Continuous-/real-valued** (**Regression problem**). Example: when y is the price of a stock, price of a house, USD/rupee conversion rate, etc.

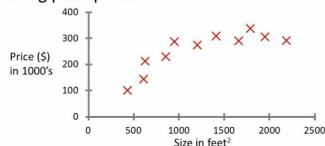
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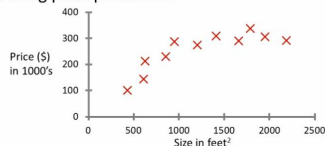
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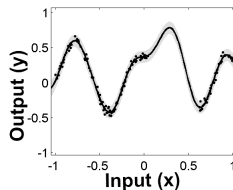
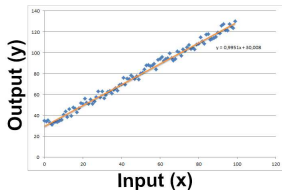
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- Many other variants (structured-prediction, multi-label learning, ordinal regression, ranking, etc.), depending on the type of label y

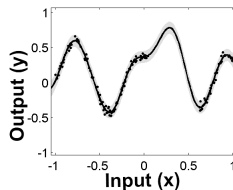
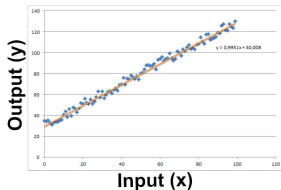
Supervised Learning: Pictorially

- Regression (linear/nonlinear): fitting a line/curve

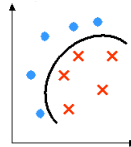
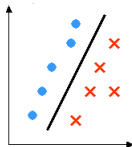


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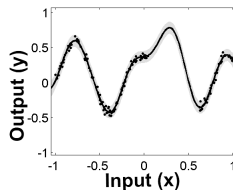
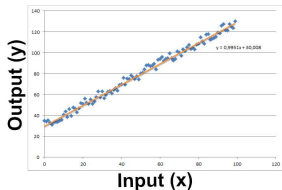


- Classification (linear/nonlinear): finding a separator

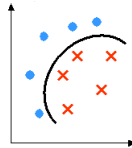
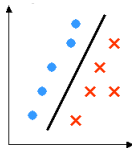


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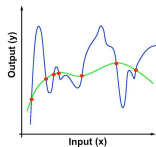
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- Generalization is crucial (must do well on test data)

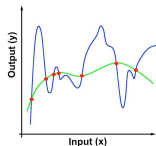
Generalization

- Simple hypotheses/rules are preferred over more complex ones

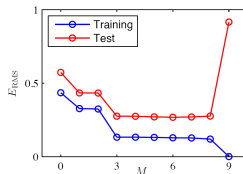
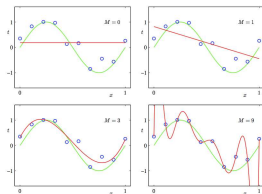


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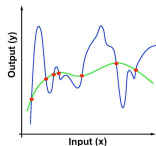


- Simple hypotheses/rules tend to generalize better

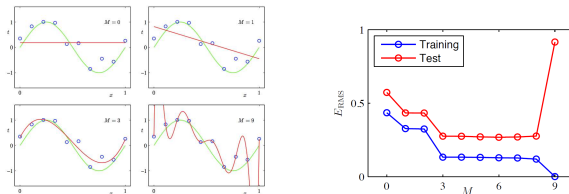


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- Desired: hypotheses that are not too simple, not too complex

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- Goal: Learn the *intrinsic structure* in the data.

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 - Data clustering (grouping similar things together)

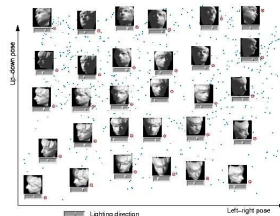
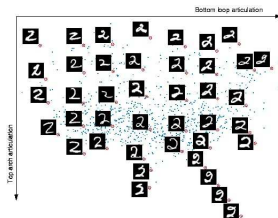


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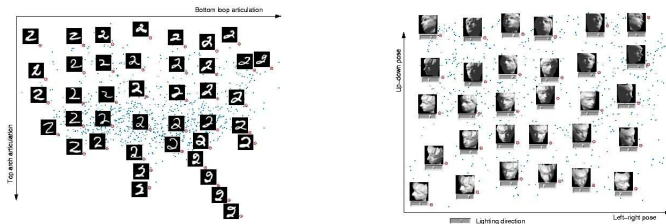


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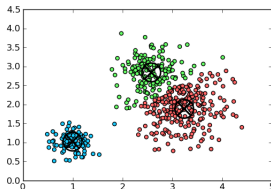
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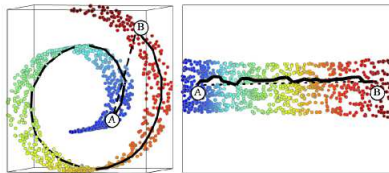
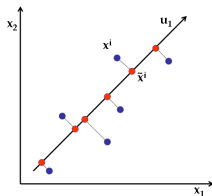
- Also very useful for summarizing/compressing data. Often also used as a preprocessing step for many supervised learning algorithms (e.g., to extract good features, to speed up the algorithms, etc.)

Unsupervised Learning: Pictorially

- Clustering: Find some “centers” and assign each data point to its “closest” center



- Dimensionality reduction: Find a lower-dimensional subspace that the data approximately lives on



Other popular Machine Learning paradigms

Semi-supervised Learning

- Learning with labeled+unlabeled data

Semi-supervised Learning

- Learning with labeled+unlabeled data
- Why is Semi-supervised Learning useful?

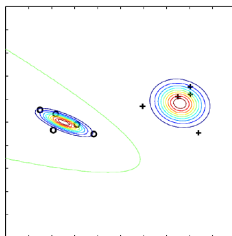
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- Why is Semi-supervised Learning useful?
 - Labeled data is expensive. Unlabeled data comes (almost) for free!

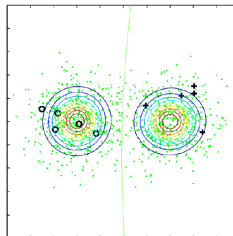
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 - Unlabeled data can provide valuable information about the distribution of data (e.g., where might the **low-density regions** or the class separator lie)

only labeled data



with unlabeled data



from [Semi-Supervised Learning, ICML 2007 Tutorial; Xiaojin Zhu]

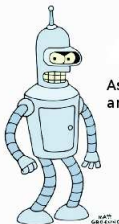
Active Learning

- The learner can interactively ask for labels of **most informative examples**



raw unlabeled data

x_1, x_2, x_3, \dots



Assumes some small
amount of initial labeled training data

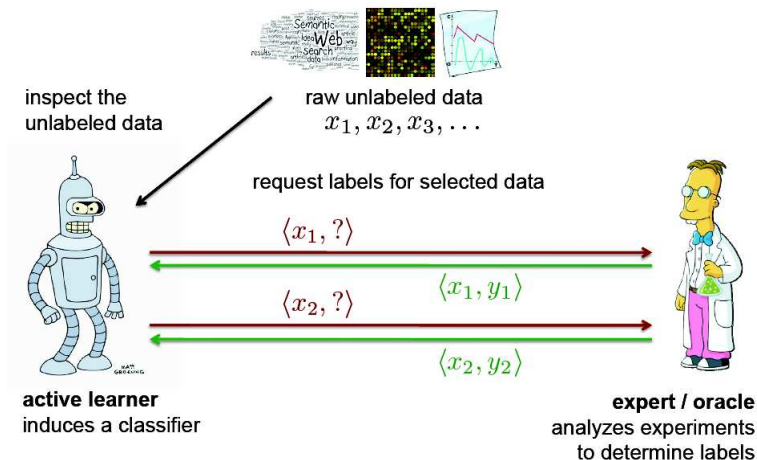
active learner
induces a classifier



expert / oracle
analyzes experiments
to determine labels

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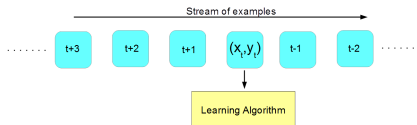
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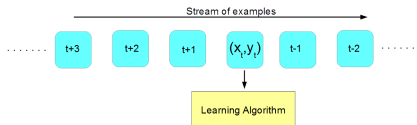
- Learning with one example (or a small minibatch of examples) at a time



Some Other Learning Paradigms

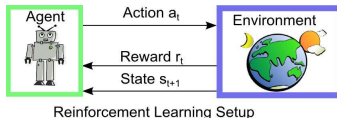
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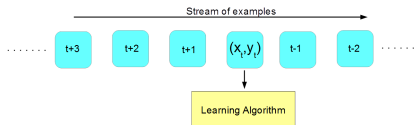
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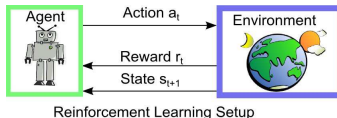
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- **Transfer/Multitask Learning**

- Leveraging knowledge of solving one problem to solve a new problem

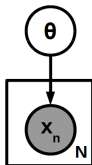


On to Probabilistic Machine Learning..

Machine Learning via Probabilistic Modeling

- Assume data $\mathbf{X} = \{\mathbf{x}_n\}_{n=1}^N$ generated from a probability distribution $p(\mathbf{x}|\theta)$, in an i.i.d. (independent and identically distributed) fashion

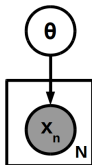
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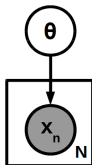


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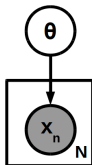


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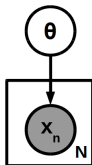


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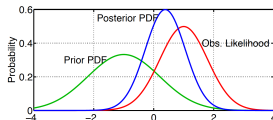


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- Variations of this general view subsume most machine learning problems
 - Regression, classification, clustering, dimensionality reduction, etc.

Parameter Estimation

- Can use Bayes rule to estimate the **posterior distribution** over parameters

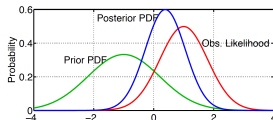
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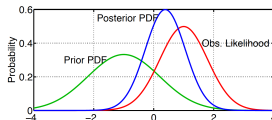


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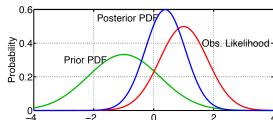
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





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- Maximum-a-Posteriori (MAP) estimation

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Some common probability distributions

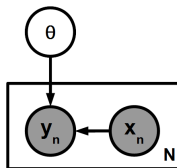
<u>Distribution</u>	<u>Domain</u>	<u>Picture</u>	<u>Parametric Form</u>
Binomial	Binary		$Bin(x N, \theta) \propto \theta^n (1 - \theta)^{N-n}$
Multinomial	K classes		$Mult(\bar{x} \bar{\theta}) \propto \prod \theta_k^{x_k}$
Beta	$[0, 1]$		$Beta(\theta \alpha, \beta) \propto \theta^{\alpha-1} (1 - \theta)^{\beta-1}$
Gamma	$[0, \infty)$		$Gam(x a, b) \propto x^{a-1} \exp(-bx)$
Dirichlet	Simplex		$Dir(\bar{\theta} \bar{\alpha}) \propto \prod \theta_k^{\alpha_k-1}$
Gaussian	Reals		$Nor(x \mu, \sigma^2) \propto \exp(-(x - \mu)^2 / 2\sigma^2)$

Some Examples of Probabilistic Modeling in Machine Learning

Probabilistic Supervised Learning

- Consider regression/classification. Training data $\{(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_N, \mathbf{y}_N)\}$
- Goal: Learn a function to predict **outputs \mathbf{y}** from **inputs \mathbf{x}**
- Model the output/response/label as a probability distribution

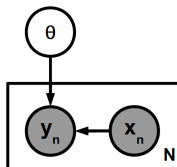
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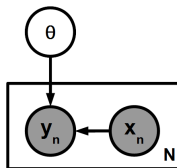


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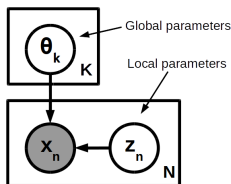


- Learning involves estimating the parameter θ given data $\{\mathbf{x}_n, \mathbf{y}_n\}_{n=1}^N$
- Can now make **probabilistic predictions** for new data \mathbf{x}_* using θ

$$p(\mathbf{y}_*|\mathbf{x}_*, \theta) \quad \text{or} \quad p(\mathbf{y}_*|\mathbf{x}_*)$$

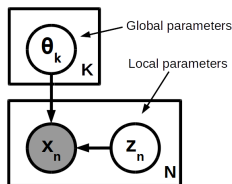
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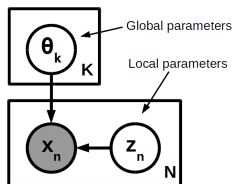
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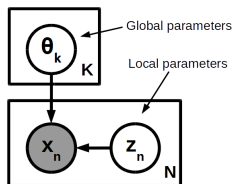
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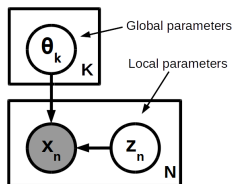
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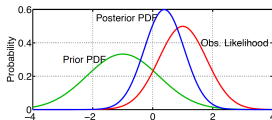
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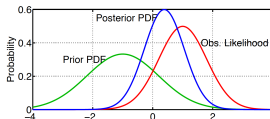
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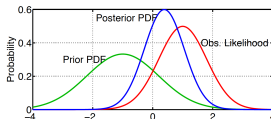


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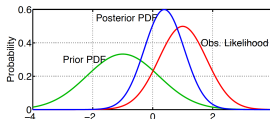
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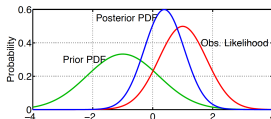
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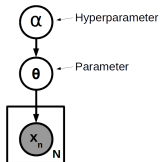
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- Can **generate** (synthesize) data by simulating from the data distribution

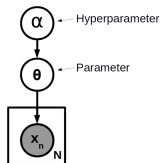
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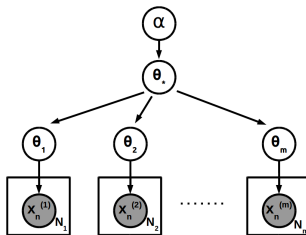


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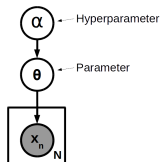


- Simple models can be neatly combined to solve complex problems

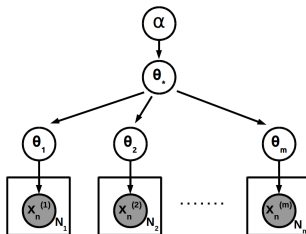


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- Many other benefits. Highly recommended to read this article from Nature:
http://www.cse.iitk.ac.in/users/piyush/courses/pml_winter16/nature14541.pdf

Course Outline

- Basics of probabilistic modeling and inference
- Probabilistic models for:
 - Regression and classification
 - Clustering
 - Dimensionality reduction
 - Matrix factorization and matrix completion
 - Time-series data modeling
- Bayesian learning and approximate inference
- Deep Learning
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Next class: Maths refresher. Common probability distributions and their properties