Course Logistics and Introduction

Piyush Rai

Probabilistic Machine Learning (CS772A)

Aug 1, 2017

Course Logistics

- **Course name:** Probabilistic Machine Learning (CS772A) - “PML”
- **Timing and Venue:** Tue/Th 6:00-7:30pm, RM-101
- **Instructor:** Piyush Rai (Email: piyush@cse.iitk.ac.in; please prefix email subject with CS772A)
- **Instructor Office Hours:** Wednesday 11:00-12:00pm (KD-319), or by appointment.

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- **Auditing?** Please let me know your email id to be added to the mailing list. You may also submit homeworks and appear for exams (we'll try to grade but it is not guaranteed)

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- 5 homework assignments: 30%
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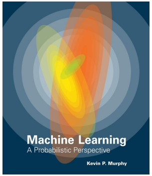

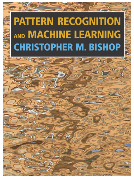

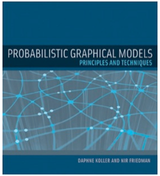

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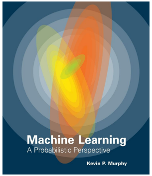

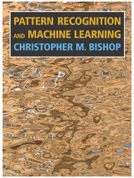

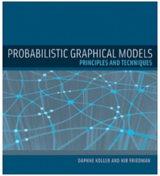

- Several other monographs on some specific topics will be provided for readings

Background Expected (Important)

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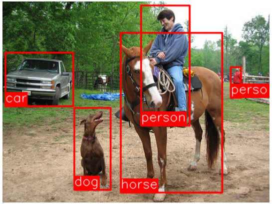
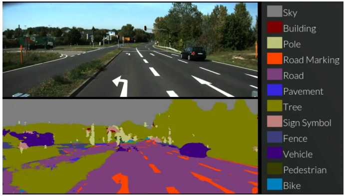
- Other things that will lead to punishment
  - Use of unfair means in the exams
  - Fabricating experimental results in assignments/project

Machine Learning 101

What is Machine Learning?

- Machines trying to make sense of data by "looking" at the data (and making decisions)





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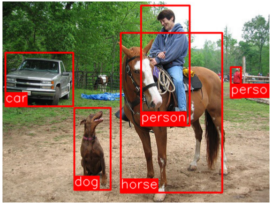
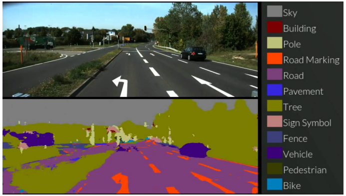


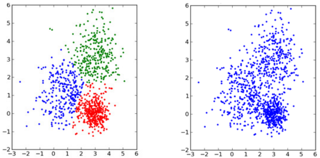


- The rules behind these decisions are not hard-coded but "inferred" from the (training) data
- Important: The rules must "generalize" to future (unseen) data

(Pic credits: kdnuggets.com, Girshick et al, CVPR 2014)

How Machines Learn?

- Primarily via one of the two ways
  - Learning with Supervision (*a.k.a.* "Supervised" Learning)
  - Learning without Supervision (*a.k.a.* "Unsupervised" Learning)



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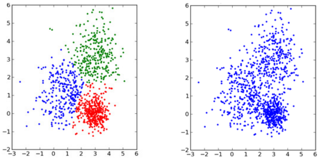

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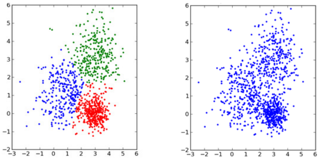

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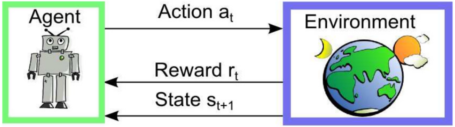
- Note: Many other learning paradigms exist (e.g, Learning through interaction)



Supervised Learning

- Given: Training data $\mathcal{D}$ in form of N input-output pairs $\{(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_N, \boldsymbol{y}_N)\}$
- Goal: Learn a function $f : \boldsymbol{x} \mapsto \boldsymbol{y}$ that can predict the output $\boldsymbol{y}_*$ for a new test input $\boldsymbol{x}_*$

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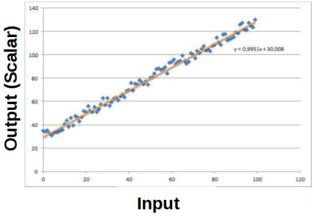
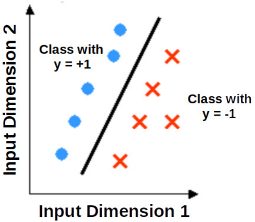
- Some examples: Regression (scalar-valued $\boldsymbol{y}$), Classification (discrete-valued y)

(Linear) Regression



(Binary) Classification



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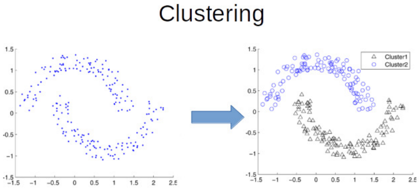

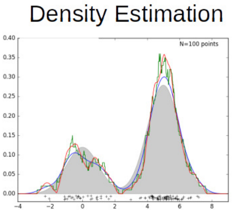

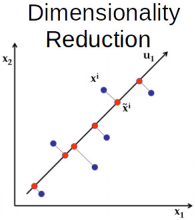

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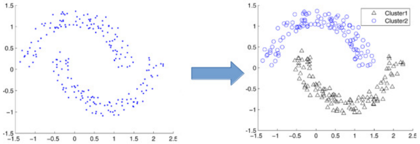
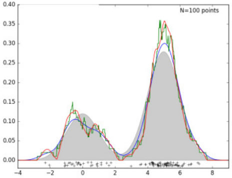
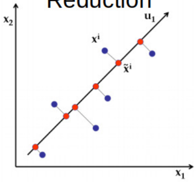


Density Estimation



Dimensionality Reduction



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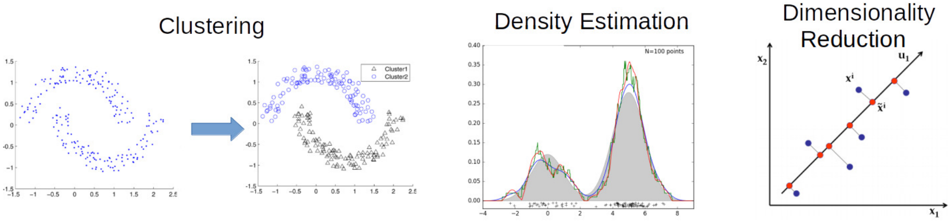
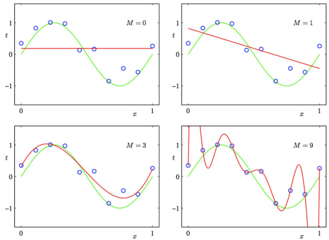
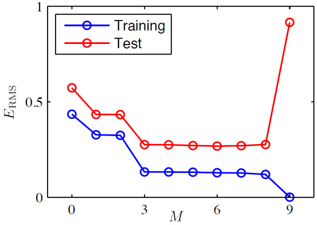


- Note: Unsupervised Learning is also related to "Data Compression"
- **Note:** Almost any ML problem (even supervised!) can be framed as a density estimation problem! As we will see, the probabilistic view of ML makes this connection even more explicit.

Overfitting vs Generalization

- Simple hypotheses/rules are preferred over more complex ones
- Reason: We care about future performance on test data, rather than the training data





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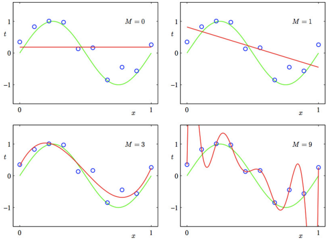

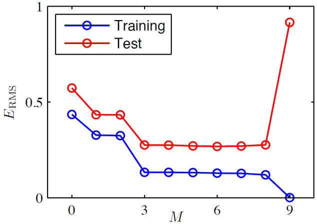

- Desired: hypotheses that are not too simple, not too complex

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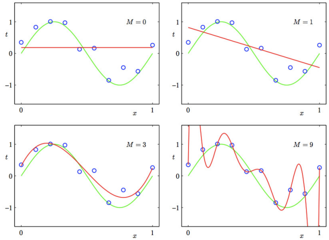

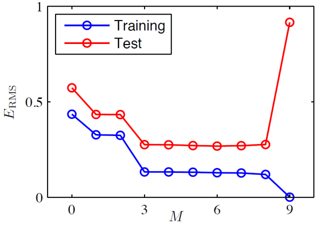

- Desired: hypotheses that are not too simple, not too complex
- ML algorithms use *regularization* to achieve this

Probabilistic Machine Learning

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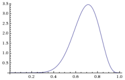

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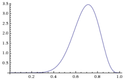

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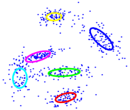

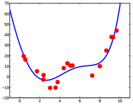

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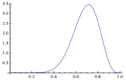

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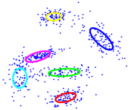
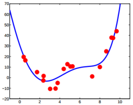
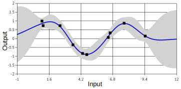




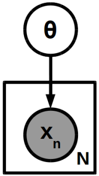
- Predictions made by the model may have uncertainty



Modeling Data Probabilistically

- Assume data $\mathbf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ generated from a probabilistic model with unknown parameters θ

$$\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \sim p(\boldsymbol{x}|\theta)$$



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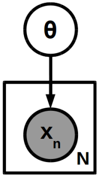

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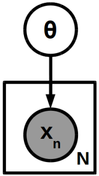

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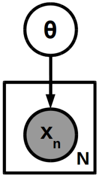

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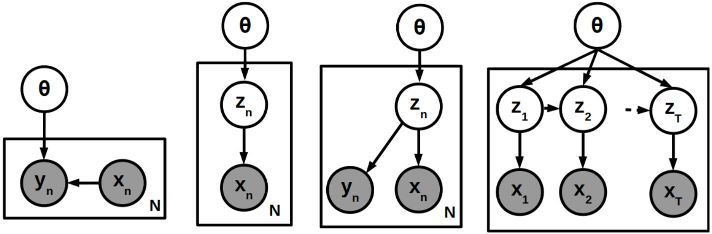
- Can use the learned model to make predictions
  - E.g., the probability $p(\boldsymbol{x}_*|\theta)$ of a new input $\boldsymbol{x}_*$ under this model

Modeling Data Probabilistically

- This basic problem set-up can be generalized in various ways



A Simple Supervised Learning Model | A Latent Variable Model for Unsupervised Learning | A Latent Variable Model for Supervised Learning | A Latent Variable Model for Sequential Data

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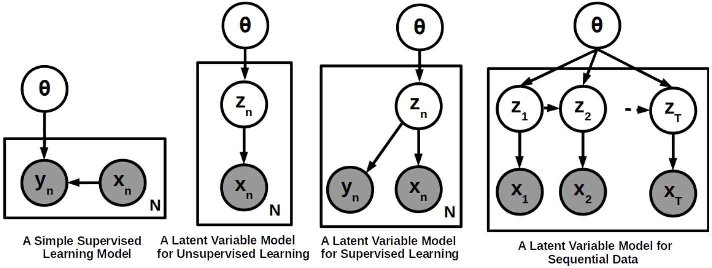

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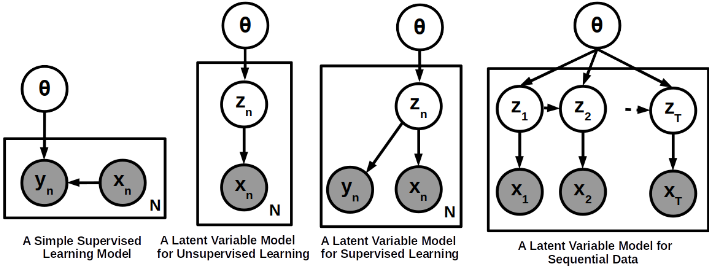

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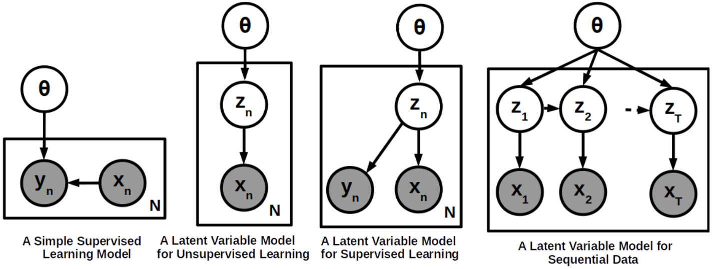

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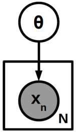
Modeling Data Probabilistically

- Specification of probabilistic models requires two key ingredients: Likelihood and prior



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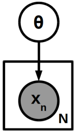

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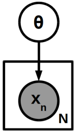

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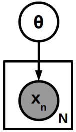

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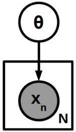
- Domain knowledge can help in the specification of the likelihood and the prior

Parameter Estimation/Inference in Probabilistic Models

- Perhaps the simplest way is to find θ that makes the observed data most likely or most probable



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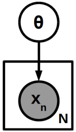

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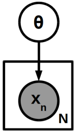

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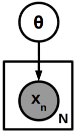

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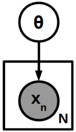

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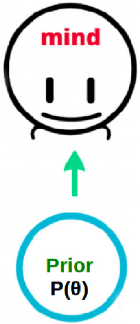
- We will study both point estimation and Bayesian inference methods (and hybrids!)

Bayesian Inference

- Bayesian inference fits naturally into an "online" learning setting



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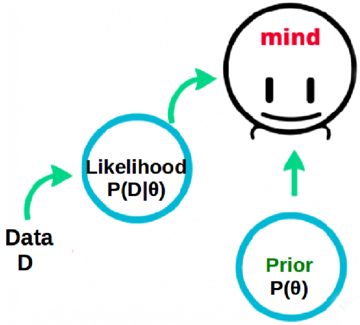

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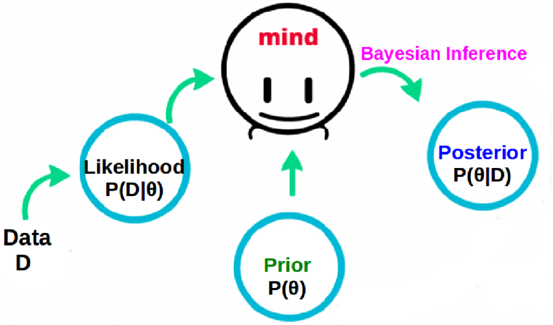

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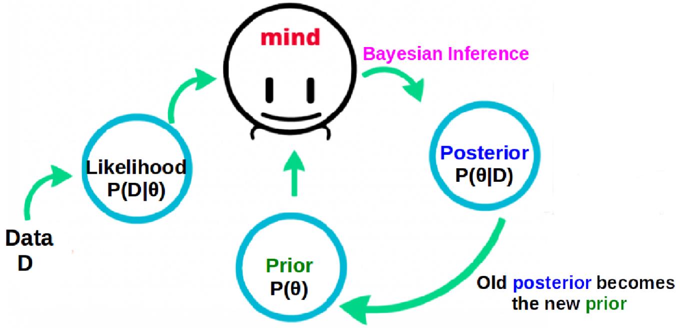

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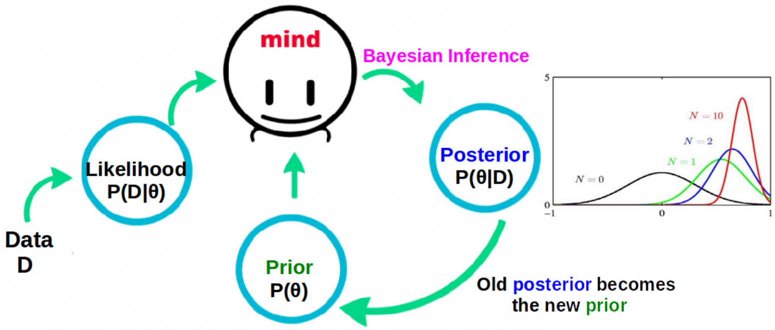

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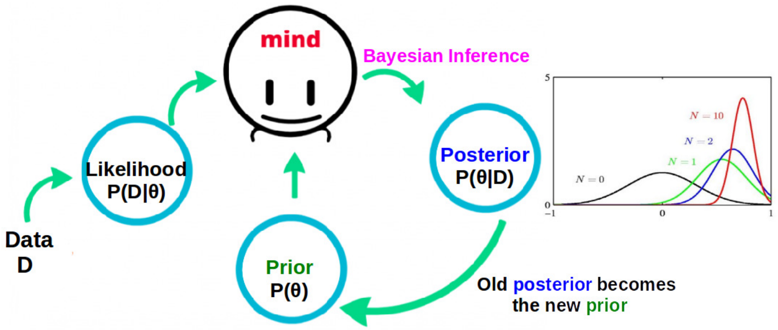
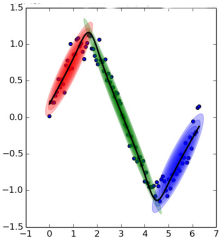


- Our belief about θ keeps getting updated as we see more and more data

Some Other Benefits of the Probabilistic Approach

Modular Construction of Complex Models

- Can easily construct combinations of multiple simple probabilistic models to learn complex patterns
- An example: Can perform nonlinear classification using a mixture of linear classifiers
  - It is a simple yet powerful combination of two models - one that performs clustering of the data and the other that learns a linear classifier within each cluster (both learned jointly)



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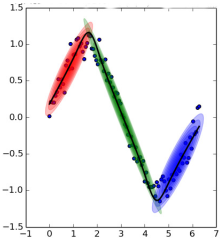
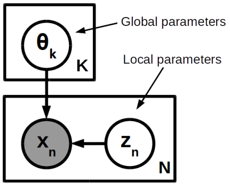


- More generally, these are called "mixture of experts" models

Generative Models

- Generative models of data can be naturally specified in a probabilistic framework



- Each data point $\boldsymbol{x}_n$ is associated with latent variables $\boldsymbol{z}_n$
- Latent variables can be used a compact representation or an "encoding" of the data
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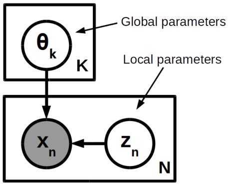

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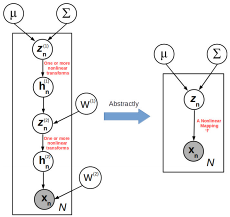
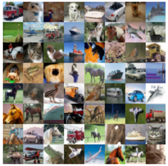
- Can also use the latent variables to infer missing data or relevance of each data point

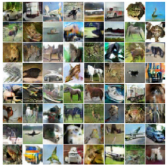
(Deep) Generative Models

- Deep Generative Models for extremely popular nowadays (e.g., Variational Auto-encoders and Generative Adversarial Networks)



- Once learned, these models can also synthesize realistic looking "new" data from random $\boldsymbol{z}$'s


Real images (CIFAR-10)


Generated images

Averaging Over Posterior Distribution

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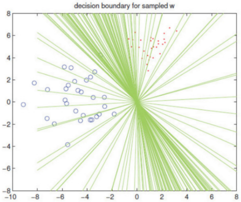
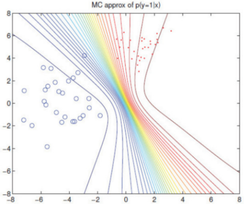
- Averaging leads to more robust predictions (and prevents overfitting)





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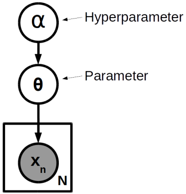

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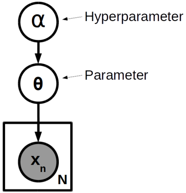

- The probabilistic approach enables learning the hyperparam. from data (without cross-validation)

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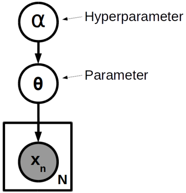

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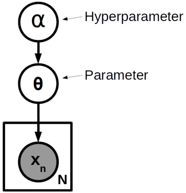

- The probabilistic approach enables learning the hyperparam. from data (without cross-validation)
  - Can put priors on the hyperparameters and infer the posterior distribution
  - Can do point estimation for hyperparameters by maximizing the marginal likelihood

$$\hat{\alpha} = \arg\max_{\alpha} \log P(\mathbf{X}|\alpha)$$

Model Comparison

- Suppose we have a number of models to choose from
- Let's compute the posterior probability of each candidate model, again using Bayes rule

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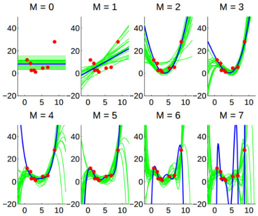

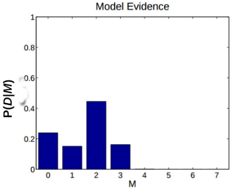

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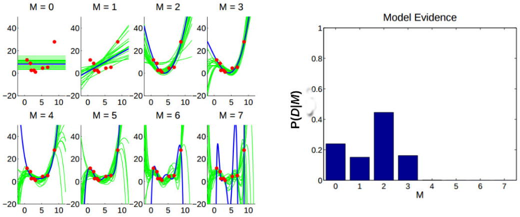
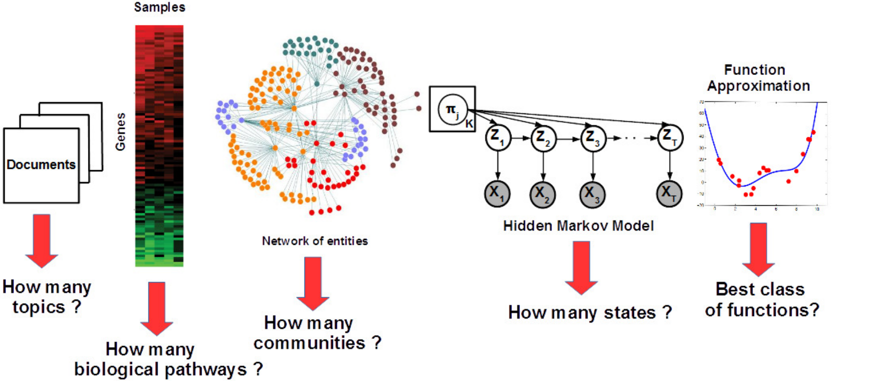


- It doesn't require a cross-validation set (can be done even for unsupervised learning problems)

Nonparametric Bayesian Modeling

- **Nonparametric Bayesian Modeling:** A principled way to learn "right" model size/complexity



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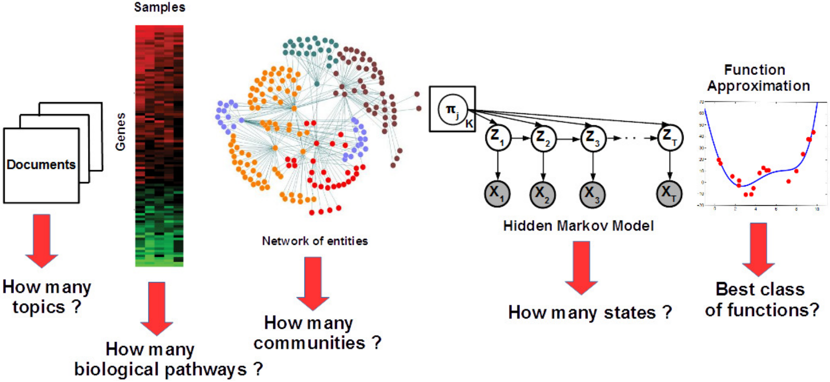

- The model size can grow with data (especially desirable for online learning settings)

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- Other advanced topics based on students' interest

Course Goals

- Learn the basics of probabilistic modeling of data
- Learn how to formulate an ML problem as a probabilistic model
- Learn how to do inference for estimating the unknowns in the model
- Learn how to implement such models (both from scratch, as well as using support from some existing software frameworks)
- Use the course project to reinforce the topics you learn in the class, and explore other topics beyond what is covered in the class

Announcement

- Need to re-schedule (prepone) the Aug 8 lecture to Aug 5 (6pm RM-101)
- Need to re-schedule (postpone) the Aug 10 lecture to Aug 14 (6pm RM-101)
- Apologies for the re-schedule. Just a one-time thing.
- A probability refresher tutorial on Aug 8 by one of the TAs (6pm RM-101)