Probabilistic Machine Learning and Bayesian Modeling

Piyush Rai

SIGML-IITK: Machine Learning Research Day

August 28, 2016

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- What data looks like: Modeled by a likelihood function $p(\mathbf{x}|\theta)$
 - $\bullet\,$ Measures data fit (or "loss") w.r.t. the given parameter $\theta\,$
- What parameters look like: Modeled by a prior distribution $p(\theta)$
 - $\bullet\,$ Also corresponds to imposing a regularizer over θ

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Learning as Optimization

Learning as (Bayesian) Inference

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• Parameter θ is a fixed unknown

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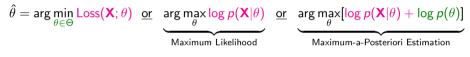


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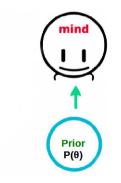


Learning as (Bayesian) Inference

- Treat the parameter θ as a random variable with a prior distribution $p(\theta)$
- Infer the full posterior distribution over the parameters using Bayes rule

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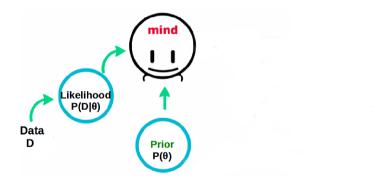
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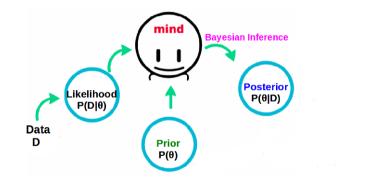
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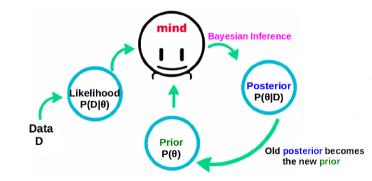
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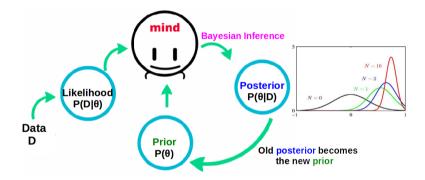
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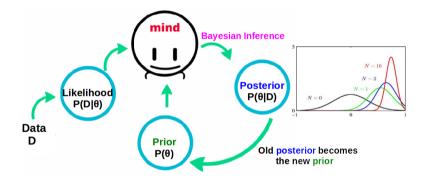
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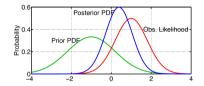
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A naturally "online" learning setting

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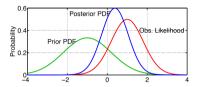
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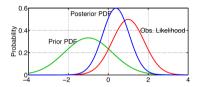
• Can make prediction y_* for test data x_* by averaging over the posterior of θ

$$\underbrace{p(y_*|x_*, X, Y)}_{\text{predictive posterior}} = \int p(y_*|x_*, \theta) p(\theta|X, Y) d\theta$$

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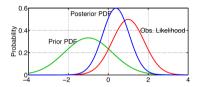
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- Less risk of overfitting since we aren't "fitting" any single parameter to the data
- Can also use **uncertainty info** in the parameter posterior or predictive posterior to decide which future observations to acquire next (also known as active learning)

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- Sequential data acquisition or "active learning"
- Consider a linear regression task:
 - Can check confidence of the learned model on the label of a test example

$$p(y|x, \theta) = \text{Normal}(y|\theta^{\top}x, \sigma^2)$$
 Likelihood
 $p(\theta|\lambda) = \text{Normal}(\theta|0, \lambda^2)$ Prior

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$p(heta \lambda)$	=	$Normal(heta 0,\lambda^2)$	Prior
$p(\theta Y, \mathbf{X})$	=	$Normal(heta \mu_ heta, \mathbf{\Sigma}_ heta)$	Parameter posterior

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$p(y_* x_*, Y, \mathbf{X})$	=	$Normal(y_* \mu_*,\sigma_*^2)$	Predictive posterior
μ_*	=	$\mu_{\theta}^{\top} \boldsymbol{x}_{*}$	Predictive mean
σ_*^2	=	$\sigma^2 + \boldsymbol{x}_*^{\top} \boldsymbol{\Sigma}_{\theta} \boldsymbol{x}_*$	Predictive variance

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• Can now choose which observations to acquire next for updating the model

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• Consider "black-box" optimization, i.e., optimizing a function whose form is not known and/or derivatives can't be computed (only the function's values can be measured at a small set of points)

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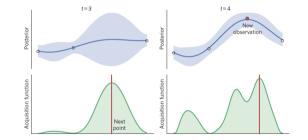
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- Bayesian Optimization: Simultaneously learn the function while finding its optima

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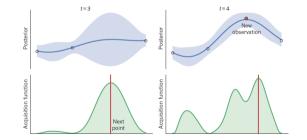
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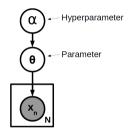


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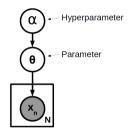
• Many applications in "explore and exploit" style problems

• Hierarchical model construction: parameters can depend on hyperparameters



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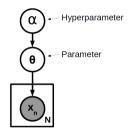
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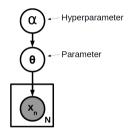
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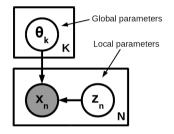
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- Examples: Learning the sparsity hyperparameter in sparse regression, learning kernel hyperparameters in kernel methods, and many unsupervised learning problems

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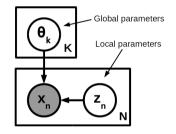
• Can do generative modeling using latent variables that "explain" data



• For each data point x_n , we can learn a compact "descriptor" feature representation z_n

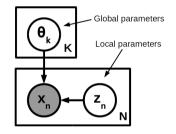
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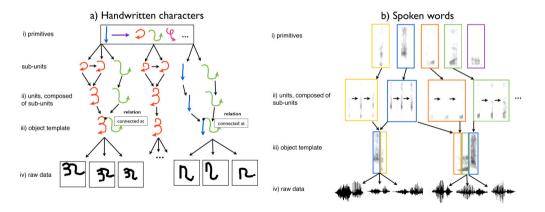
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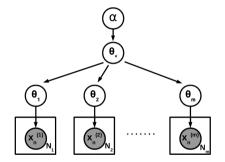


- For each data point x_n , we can learn a compact "descriptor" feature representation z_n
- Used in many problems, especially unsupervised learning: Gaussian mixture model, probabilistic principal component analysis, factor analysis, topic models, deep feature learning, etc.
- Can also use the latent variables to infer missing data or relevance of each data point

• Generative modeling also enables synthesizing new data from the learned model (useful in diagnosing whether the learned model is sensible or not, especially in unsupervised learning)



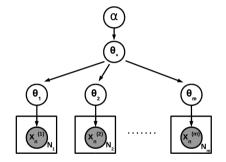
• Simple models can be neatly combined to solve more complex problems



• Allows joint learning across multiple data sets (known as multitask learning or transfer learning)

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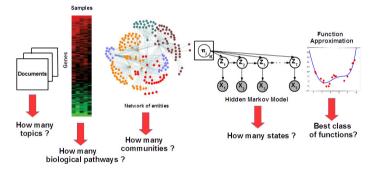


• Allows joint learning across multiple data sets (known as multitask learning or transfer learning)

• Enables different but related models to "share statistical strength"

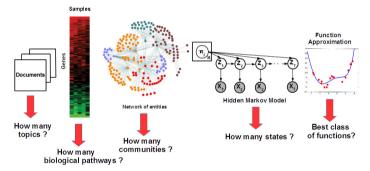
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• Nonparametric Bayesian Modeling: A principled way to learn "right" model size/complexity



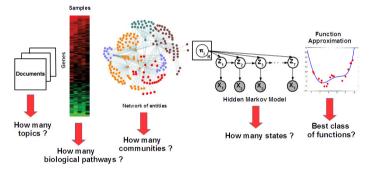
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- The model size can grow with data (especially desirable for online learning settings)
- A very elegant modeling paradigm: Can be seen as an infinite limit of finite models

Piyush Rai (CSE, IIT Kanpur)

• Recall the basic principle of Bayesian inference

$$P(heta|\mathbf{X}) = rac{P(\mathbf{X}| heta)P(heta)}{P(\mathbf{X})} \propto \mathsf{Likelihood} imes \mathsf{Prior}$$

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 - Rather, these problems are characterized by the massive number of parameters to be learned
 - However, in these problems, the amount of data available for learning each parameter is very small (e.g., a massive user-ratings data set usually has very few ratings per user)
- Therefore modeling/quantifying parameter uncertainty makes all the more sense

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- Designing flexible and scalable Bayesian models for specific problems, e.g., deep learning
 - Flexibility via nonparametric Bayesian models (to adapt model sizes as warranted by data)
 - Scalability via online Bayesian inference that mirrors online optimization

$$\theta' = \theta_t + \frac{\epsilon_t}{2} \left(\nabla \log \pi_0(\theta_t) + \frac{N}{m} \sum_{n=1}^m \nabla \log \pi(x_n \mid \theta_t) \right) + \eta_t$$

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- Developing automated Bayesian modeling and inference methods

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- Exploring connections to prevalent concepts in other "hot" areas in ML, e.g.,
 - Dropout in Deep Learning equivalent to doing approximate Bayesian inference
- Developing automated Bayesian modeling and inference methods
 - Probabilistic Programming: Express probabilistic models via computer programs and perform automatic inference (check out **Stan**)

Some Resources

On Probabilistic/Bayesian Modeling

- Book: Pattern Recognition and Machine Learning (Chris Bishop)
- Book: Machine Learning A Probabilistic Perspective (Kevin Murphy)
- Introductory Paper: "Bayesian Inference: An Introduction to Principles and Practice in Machine Learning" (Mike Tipping) http://www.miketipping.com/papers/met-mlbayes.pdf
- Introductory Paper: "Probabilistic machine learning and artificial intelligence" (Zoubin Ghahramani) http://www.nature.com/nature/journal/v521/n7553/full/nature14541.html
- "Roadmap" to learning about Bayesian learning (from Metaacademy): https://www.metacademy.org/roadmaps/rgrosse/bayesian_machine_learning

On Bayesian Optimization

• Taking the Human Out of the Loop: A Review of Bayesian Optimization (Shahriari et al, 2015) https://www.cs.ox.ac.uk/people/nando.defreitas/publications/BayesOptLoop.pdf

On Probabilistic Programming

• Check out Stan http://mc-stan.org/

On Nonparametric Bayesian Learning

 A brief tutorial: A tutorial on Bayesian nonparametric models (Gershman & Blei, 2012) http://web.mit.edu/sjgershm/www/GershmanBlei12.pdf

On Gaussian Processes

- Book: Gaussian Processes for Machine Learning (freely available online)
- MATLAB Package GPML: http://www.gaussianprocess.org/gpml/code/matlab/doc/
- MATLAB Package GPStuff: http://research.cs.aalto.fi/pml/software/gpstuff/

Thanks! Questions?

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