



#### Lecture 8: When Models Meet Data

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Mathematics for Machine Learning
https://yung-web.github.io/home/courses/mathml.html
KAIST EE

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(1) Data, Models, and Learning

(2) Models as Functions: Empirical Risk Minimization

(3) Models as Probabilistic Models: Parameter Estimation (ML and MAP)

(4) Probabilistic Modeling and Inference

(5) Directed Graphical Models

(6) Model Selection

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#### Roadmap



Data, Models, and Learning



- (1) Data, Models, and Learning
- (2) Models as Functions: Empirical Risk Minimization
- (3) Models as Probabilistic Models: Parameter Estimation (ML and MAP)
- (4) Probabilistic Modeling and Inference
- (5) Directed Graphical Models
- (6) Model Selection

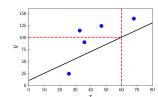
- Three major components of a machine learning system
  - 1. Data:  $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n), \dots, (\mathbf{x}_N, y_N)\}$
  - $2. \ \ Models: deterministic functions or probabilistic models$
- 3. Learning: Training, and prediction/inference
- Good machine learning models: Perform well for unseen (untrained) data
- Machine learning algorithm: training and prediction

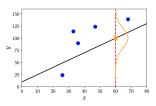


- Tabular format or not, numerical or not, good feature extraction etc.
- Assume that data is given as D-dimensional vector  $\mathbf{x}_n$  of real numbers, each called features, attributes, or covariates.
- Dataset: consisting of data points or examples  $\{x_1, x_2, \ldots, x_N\}$
- In supervised learning,  $\{(x_1, y_1), \dots, (x_n, y_n), \dots, (x_N, y_N)\}$ , where  $y_n$  is the label (or target, response variable, or annotation).
- Better representation of data as vectors
  - $\circ$  finding lower-dimensional approximations of the original feature vector (e.g., PCA via SVD or EVD)
  - using nonlinear higher-dimensional combinations of the original feature vector (e.g., feature map and kernel)

Now, the business of constructing a predictor

- Models as functions
  - $\circ f: \mathbb{R}^D \mapsto \mathbb{R}.$
  - Example.  $f(\mathbf{x}) = \boldsymbol{\theta}^\mathsf{T} \mathbf{x} + \theta_0$ , Unknown parameter:  $\boldsymbol{\theta}, \theta_0$
- Models as probabilistic models
  - model our uncertainty due to the observation process and our uncertainty in the parameters of our model
  - predictors should be able to express some sort of uncertainty via probabilistic models
  - Parameters: parameters of a chosen probabilistic model (e.g., mean and variance of Gaussian)





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#### Learning Algorithms



Roadmap



Three algorithmic phases

- (1) Prediction or inference: via function or probabilitic models
- (2) Training or parameters estimation
  - fixed parameter assumption (non-probabilistic) or Bayesisan approach (probabilistic)
  - o non-probabilistic: e.g., empirical risk minimization
  - o probabilistic: e.g., ML (Maximum Likelihood), MAP (Maximum A Posteriori)
  - o cross-validation: simulation of performing for unseen data
  - o regularization/prior: balancing models between training and unseen data
- (3) Hyperparameter tuning or model selection

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- Predictor as a function
- Given  $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n), \dots, (\mathbf{x}_N, y_N)\}$ , estimate a predictor  $f(\cdot, \theta) : \mathbb{R}^D \to \mathbb{R}$
- Find a good parameter  $\theta^*$ , such that  $f(\mathbf{x}_n, \theta^*) = \hat{y}_n \approx y_n$ , for all  $n = 1, \dots, N$
- Example. Affine function: By adding the unit feature  $x^{(0)} = 1$  and  $\theta_0$ , i.e.,  $\mathbf{x}_n = \begin{bmatrix} 1, x_n^{(1)}, \dots, x_n^{(D)} \end{bmatrix}^\mathsf{T}$ ,  $\boldsymbol{\theta} = \begin{bmatrix} \theta_0, \theta_1, \dots, \theta_D \end{bmatrix}^\mathsf{T}$

$$f(\mathbf{x}_n, \boldsymbol{\theta}) = \boldsymbol{\theta}^\mathsf{T} \mathbf{x}_n = \theta_0 + \sum_{d=1}^D \theta_d x_n^{(d)}$$

• Example. Neural network: Complex non-linear function

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- Training set:  $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n), \dots, (\boldsymbol{x}_N, y_N)\}$ , an example matrix<sup>1</sup>  $\boldsymbol{X} := [\boldsymbol{x}_1, \dots, \boldsymbol{x}_N]^\mathsf{T} \in \mathbb{R}^{N \times D}$ , a label vector  $\boldsymbol{y} := [y_1, \dots, y_N]^\mathsf{T}$ ,
- Average loss, empirical risk

$$R_{\mathsf{emp}}(f, \boldsymbol{X}, \boldsymbol{y}) = \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, \hat{y}_n)$$

- · Goal: Minimizing empirical risk
- Example. The squared loss function  $\ell(y_n, \hat{y}_n) = (y_n \hat{y}_n)^2$  leads to:

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \frac{1}{N} \| \boldsymbol{y} - \boldsymbol{X} \boldsymbol{\theta} \|^2$$

- Question. Ultimgate goal: Minimizing expected risk (for unseen data)  $R_{\text{true}} = \mathbb{E}_{\mathbf{x},y}[\ell(y, f(\mathbf{x}))]$ ?
- <sup>1</sup>In other chapters, we often use  $D \times N$  example matrix by defining it as  $\mathbf{X} := [x_1, \dots, x_N]$ . L10(4)

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#### Overfitting and Regularization



Cross-Validation for Generalization Performance

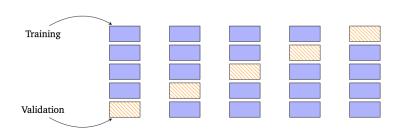
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- The predictor fits too closely to the training data and does not generalize well to new data
- Need to somehow bias the search for the minimizer of empirical risk by introducing a penalty term
- Regularization: compromise between accurate solution of empirical risk minimization and the size or complexity of the solution.
- Example. Regularized Least Squares

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \frac{1}{N} \| \boldsymbol{y} - \boldsymbol{X} \boldsymbol{\theta} \|^2 + \lambda \| \boldsymbol{\theta} \|^2$$

 $\|\theta\|^2$ : regularizer,  $\lambda$ : regularization parameter





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- Idea: define a function of the parameters called likelihood function.
- Negative log-likelihood for data x and a family of probability densities  $\mathbb{P}(x \mid \theta)$  parameterized by  $\theta$ :

$$\mathcal{L}_{\mathbf{x}}(\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}) := -\log \mathbb{P}(\mathbf{x} \mid \boldsymbol{\theta})$$

- $\mathcal{L}(\theta)$ : how likely a particular setting of  $\theta$  is for the observations x.
- MLE: Find  $\theta$  such that  $\mathcal{L}(\theta)$  is minimized (i.e., likelihood is maximized)

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#### MLE: Supervised Learning



MAP (Maximum A Posteriori)



- The set of iid examples  $(x_1, y_1), \dots, (x_N, y_N)$
- $\mathcal{X} = \{x_1, ..., x_N\}$  and  $\mathcal{Y} = \{y_1, ..., y_N\}$
- Negative log-likelihood

$$\mathcal{L}(oldsymbol{ heta}) = -\log \mathbb{P}(\mathcal{Y} \mid \mathcal{X}, oldsymbol{ heta}) = \sum_{n=1}^{N} \log \mathbb{P}(y_n \mid oldsymbol{x}_n, oldsymbol{ heta})$$

• Example. Assume independent Gaussian noise  $\mathcal{N}(0, \sigma^2)$  and linear model  $y_n = \mathbf{x}_n^\mathsf{T} \boldsymbol{\theta}$  for prediction. Then,  $Y_n | (\mathbf{x}_n, \boldsymbol{\theta}) \sim \mathcal{N}(\mathbf{x}_n^\mathsf{T} \boldsymbol{\theta}, \sigma^2)$ .

$$\mathcal{L}(\boldsymbol{\theta}) = -\sum_{n=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_n - \boldsymbol{x}_n^\mathsf{T}\boldsymbol{\theta})^2}{2\sigma^2}\right) = \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \boldsymbol{x}_n^\mathsf{T}\boldsymbol{\theta})^2 - \sum_{n=1}^{N} \log \frac{1}{\sqrt{2\pi\sigma^2}}$$

- What if we have some prior knowledge about  $\theta$ ? Then, how should we change our knowledge about  $\theta$  after observing data x?
- Compute a posteriori distribution (using Bayes' Theorem) and find  $\theta$  that maximizes the distribution:

$$\max_{\boldsymbol{\theta}} \mathbb{P}(\boldsymbol{\theta} \mid \boldsymbol{x}) = \max_{\boldsymbol{\theta}} \frac{\mathbb{P}(\boldsymbol{x} \mid \boldsymbol{\theta}) \mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\boldsymbol{x})} \Longleftrightarrow \min_{\boldsymbol{\theta}} \Big( -\log \mathbb{P}(\boldsymbol{\theta} \mid \boldsymbol{x}) \Big)$$

- $\circ$  In finding the optimal  $\theta$ ,  $\mathbb{P}(x)$  can be ignored
- ML and MAP: Bridging the non-probabilistic and probabilistic worlds as it explicitly acknowledges the need for a prior distribution, yet producing a point estimate (one single parameter return).

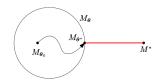
# **Model Fitting**

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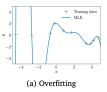
Roadmap

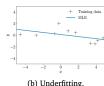


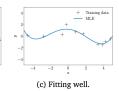
• Model class  $M_{\theta}$  vs. Right model  $M^*$ 



• Overfitting vs. Underfitting vs. Good fitting







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#### Modeling Generative Process and Probabilistic Models



#### Fully Bayesian vs. ML/MAP



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· Many machine learning tasks: prediction of future events and decision making

- Often build (probabilistic) models that describe the generative process that generates the observed data
- In probabilistic modeling, the joint distribution  $\mathbb{P}(x,\theta)$  of the observed variables x and the hidden parameters  $\theta$  encapsulate the key information
  - Given: prior  $\mathbb{P}(\theta)$  and likelihood  $\mathbb{P}(x|\theta)$
  - Joint dist. from prior and likelihood:  $\mathbb{P}(\mathbf{x}, \theta) = \mathbb{P}(\mathbf{x}|\theta)\mathbb{P}(\theta)$
  - We get: marginal likelihood  $\mathbb{P}(\mathbf{x}) = \int \mathbb{P}(\mathbf{x}, \boldsymbol{\theta}) d\boldsymbol{\theta}$  and posterior  $\mathbb{P}(\boldsymbol{\theta}|\mathbf{x}) = \frac{\mathbb{P}(\mathbf{x}, \boldsymbol{\theta})}{\mathbb{P}(\mathbf{x})}$

Given the data set  $\mathcal{X}$ , we want to predict A, i.e.,  $\mathbb{P}(A \mid \mathcal{X})$ 

• ML: Easy (high), Exact (low)

$$\mathbb{P}(A \mid \mathcal{X}) \approx \mathbb{P}(A \mid \boldsymbol{\theta}), \quad \boldsymbol{\theta} = \arg \max \mathbb{P}(\mathcal{X} \mid \boldsymbol{\theta})$$

MAP: Easy (mid), Exact (mid)

$$\mathbb{P}(A \mid \mathcal{X}) \approx \mathbb{P}(A \mid \boldsymbol{\theta}), \quad \boldsymbol{\theta} = \arg \max \mathbb{P}(\boldsymbol{\theta} \mid \mathcal{X})$$

- Fully Bayesian: Easy (low), Exact (high)
  - predictive inference, use of posterior predictive distribution, bayesian prediction
  - remove dependence on the model parameters heta

$$\mathbb{P}(A \mid \mathcal{X}) = \int \mathbb{P}(A \mid oldsymbol{ heta}) \mathbb{P}(oldsymbol{ heta} \mid \mathcal{X}) \mathrm{d}oldsymbol{ heta}$$

- Only possible by getting the full posterior distribution  $\mathbb{P}(\theta \mid \mathcal{X})$ 



• For a data set  $\mathcal{X}$ , a parameter prior  $\mathbb{P}(\theta)$ , and a likelihood function, the posterior is:

$$\mathbb{P}(oldsymbol{ heta} \mid \mathcal{X}) = rac{\mathbb{P}(\mathcal{X} \mid oldsymbol{ heta})\mathbb{P}(oldsymbol{ heta})}{\mathbb{P}(\mathcal{X})}, \quad \mathbb{P}(\mathcal{X}) = \int \mathbb{P}(\mathcal{X} \mid oldsymbol{ heta})\mathbb{P}(oldsymbol{ heta}) \, \mathrm{d}oldsymbol{ heta}$$

- Implementation hardness
  - Bayesian inference requires to solve integration, which is often challenging. In particular, a conjugate prior is not chosen, the integration is not analytically tractable.
  - Approximation techniques: MCMC (Markov Chain Monte Carlo), Laplace approximation, variational inference, expectation propagation

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- Including latent variables in the model ightarrow contributing to the interpretability of the model
- General discussions here would be applied the following examples later
  - PCA for dimensionality reduction

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Gaussian mixture models for density estimation



- In latent-variable models (LVMs)<sup>2</sup>,
  - Given: prior  $\mathbb{P}(z)$  and likelihood  $\mathbb{P}_{\theta}(x|z)$
  - $\circ$  Joint dist. from prior and likelihood:  $\mathbb{P}_{\theta}(x,z) = \mathbb{P}_{\theta}(x|z)\mathbb{P}(z)$
  - o Our interest: marginal likelihood  $\mathbb{P}_{\theta}(x)$  and posterior  $\mathbb{P}_{\theta}(z|x)$

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# LVM (2)



LVM (3): Why the posterior distribution  $\mathbb{P}_{\theta}(z|x)$ ?



- Assuming we know  $\theta$ , to generate a data sample from the model (i) sample z from  $\mathbb{P}(z)$  and (ii) sample x from  $\mathbb{P}_{\theta}(x|z)$
- Inference. computing the posterior distribution  $\mathbb{P}_{\theta}(z|x)$ :

$$\mathbb{P}_{\theta}(z|x) = \frac{\mathbb{P}_{\theta}(x,z)}{\mathbb{P}_{\theta}(x)} = \frac{\mathbb{P}_{\theta}(x,z)}{\int \mathbb{P}_{\theta}(x,z) dz}$$

• This requires to solve the sub-problem of computing the marginal likelihood of the observation:

$$\mathbb{P}_{m{ heta}}(m{x}) = \int \mathbb{P}_{m{ heta}}(m{x},m{z}) \mathrm{d}m{z}$$

- Explanation of the observation. Allows us to figure out which latent configurations could have plausibly generated the observation data samples.
- Learning of model parameters  $\theta$ . Training LVMs to estimate  $\theta$  (e.g., ML) requires  $\mathbb{P}_{\theta}(z|x)$  in its inner loops

marginal likelihood  $\mathbb{P}_{ heta}(\mathbf{x}) \Longrightarrow$  posterior distribution  $\mathbb{P}_{ heta}(\mathbf{z}|\mathbf{x}) \Longrightarrow heta_{\mathsf{ML}}$ 

 $<sup>^2</sup>$ In our note, we express the dependence on the model parameters  $\theta$  using subscript notations, e.g.,  $\mathbb{P}_{\theta}(x|z)$  rather than  $\mathbb{P}(x|z,\theta)$  to highlight the role of z.



• In ML, we need the gradient of the marginal log-likelihood. For a data sample x,

$$\nabla_{\theta} \log p_{\theta}(\mathbf{x}) = \frac{\nabla_{\theta} p_{\theta}(\mathbf{x})}{p_{\theta}(\mathbf{x})} = \frac{\int \nabla_{\theta} p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}}{p_{\theta}(\mathbf{x})} = \frac{\int p_{\theta}(\mathbf{x}, \mathbf{z}) \nabla_{\theta} \log p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}}{p_{\theta}(\mathbf{x})}$$
$$= \int p_{\theta}(\mathbf{z}|\mathbf{x}) \nabla_{\theta} \log p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

•  $\mathbb{P}_{\theta}(z|x)$  performs credit assignment over latent configurations

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#### **Graphical Models**

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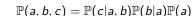
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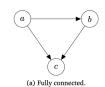
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# **Graph Semantics**



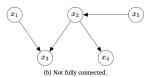
- Joint distribution of a probabilistic model: key quantity of interest, but quite complicated without structural properties
- However, there exist relations of independence, conditional independence among random variables.
- (Probabilistic) graphical models: Roughly speaking, a graph of random variables.
  - Simple ways to visualize the structure of the model
  - Insights into the structural properties, e.g., conditional independence
  - Computations for inference and learning can be expressed in terms of graphical manipulations





 $\mathbb{P}(x_1)\mathbb{P}(x_5)\mathbb{P}(x_2|x_5)\mathbb{P}(x_3|x_1,x_2)\mathbb{P}(x_4|x_2)$ 

 $\mathbb{P}(x_1, x_2, x_3, x_4, x_5) =$ 



Nodes: random variables

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- Directed edge for direct dependence: b directly depends on a:  $a \rightarrow b$
- Graph layout: factorization of the joint distribution

$$\mathbb{P}(x_1,\ldots,x_K) = \prod_{k=1}^K \mathbb{P}(x_k \mid \mathsf{Pa}_k), \quad \mathsf{Pa}_k \text{ are the parent nodes of } x_k.$$

# Example: N coin-flip experiments

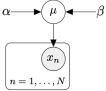


# Conditional Independence and d-Separation



 $x_1$   $x_N$ 





- (a) Version with  $x_n$  explicit.
- (b) Version with plate notation.
- (c) Hyperparameters  $\alpha$  and  $\beta$  on the latent  $\mu$ .
- Shaded nodes: observables,  $\mu$ : probability of head, a (latent) random variable
- Joint distribution

$$\mathbb{P}(x_1,\ldots,x_N\mid\mu)=\prod_{n=1}^N\mathbb{P}(x_n\mid\mu)$$

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- Question. How can we see conditional independence in the directed graphical models? For example,  $\mathcal{A} \perp \!\!\! \perp \mathcal{B} \mid \mathcal{C}$ ?
- *d*-separation
  - $\circ$  All possible trails<sup>3</sup> from any node  ${\mathcal A}$  to any node in  ${\mathcal B}$
  - Any such path is blocked if it includes any node such that either of the following is true:
    - ► The arrows on the path meet either head to tail or tail to tail at the node, and the node is in C
    - $\,\blacktriangleright\,$  The arrows meet head to head at the node, and neither the node nor any of its descendants is in  ${\cal C}$
  - If all the paths are blocked, then A is d-separated from B by C.
  - $\circ$  If *d*-separated,  $\mathcal{A} \perp \!\!\! \perp \mathcal{B} \mid \mathcal{C}$

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#### Example

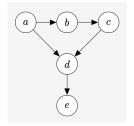


# Example in Healthcare

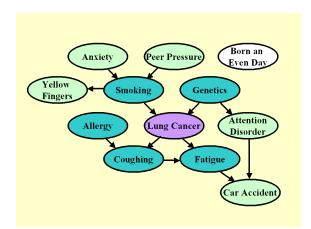


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Source: http://www.causality.inf.ethz.ch/data/LUCAS.html

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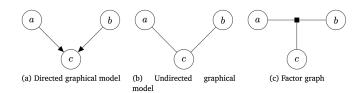
<sup>&</sup>lt;sup>3</sup>paths that ignore the direction of the arrows

# Three Types of Graphical Models



Roadmap





- Directed graphical models (or Bayesian Networks)
- Undirected graphical models (Markov Random Fields)
- Factor graphs

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# Nested Cross-Validation



Bayesian Model Selection



All labeled data All training data Test data Validation To train model

Model selection

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- Tradeoff between model complexity and data fit
- Occam's razor. Find the simplest model that explains the data resonably well.
- Test set: estimate the generalization performance
- Validation set: choose the best model

• A set of models  $\mathbf{M} = \{M_1, \dots, M_k\}$ , where each  $M_k$  has  $\theta_k$  parameters. A prior  $\mathbb{P}(M)$  on each model  $M \in \mathbf{M}$ .

$$M_k \sim \mathbb{P}(M), \quad oldsymbol{ heta}_k \sim \mathbb{P}(oldsymbol{ heta} \mid M_k), \quad \mathcal{D} \sim \mathbb{P}(\mathcal{D} \mid oldsymbol{ heta}_k)$$

• Posterior distribution  $\mathbb{P}(M_k \mid \mathcal{D}) \propto \mathbb{P}(M_k) \mathbb{P}(\mathcal{D} \mid M_k)$ , where we have the following model evidence or marginal likelihood:

$$\mathbb{P}(\mathcal{D} \mid M_k) = \int \mathbb{P}(\mathcal{D} \mid \boldsymbol{ heta}_k) \mathbb{P}(\boldsymbol{ heta}_k \mid M_k) d\boldsymbol{ heta}_k \quad (***)$$

- MAP for the model:  $M^* = \arg \max_{M_k} \mathbb{P}(M_k \mid \mathcal{D})$
- With the uniform model prior (i.e.,  $\mathbb{P}(M_k) = 1/k$ ), the MAP estimate equals to maximization of model evidence.



• Compare two probabilistic models  $M_1$  and  $M_2$ :

$$(\text{Posterior odds}) = \frac{\mathbb{P}(M_1 \mid \mathcal{D})}{\mathbb{P}(M_2 \mid \mathcal{D})} = \frac{\frac{\mathbb{P}(\mathcal{D}|M_1)\mathbb{P}(M_1)}{\mathbb{P}(\mathcal{D})}}{\frac{\mathbb{P}(\mathcal{D}|M_2)\mathbb{P}(M_2)}{\mathbb{P}(\mathcal{D})}} = \underbrace{\frac{\mathbb{P}(M_1)}{\mathbb{P}(M_2)}}_{\text{Prior odds}} \underbrace{\frac{\mathbb{P}(\mathcal{D} \mid M_1)}{\mathbb{P}(\mathcal{D} \mid M_2)}}_{\text{Bayes factor}}$$

- $\mathbb{P}(\mathcal{D} \mid M_k)$ : How well the data is predicted by the model  $M_k$
- ullet With the uniform model prior, the prior odds =1
- Computation of Bayes factor requires the complex integration (\*\*\*) in the previous slide. In this case, we rely on some approximations such as MCMC (Markov Chain Monte Carlo).

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**Review Questions** 

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1)

Questions?