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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- Three major components of a machine learning system
  1. Data: $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$

  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 $\boldsymbol{x}_n$ of real numbers, each called features, attributes, or covariates.

- Dataset: consisting of data points or examples $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$

- In supervised learning, $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$, where y_n is the label (or target, response variable, or annotation).

- Better representation of data as vectors
  - 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
  - $f : \mathbb{R}^D \mapsto \mathbb{R}$.
  - Example. $f(\boldsymbol{x}) = \boldsymbol{\theta}^\mathsf{T} \boldsymbol{x} + \theta_0$, 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)
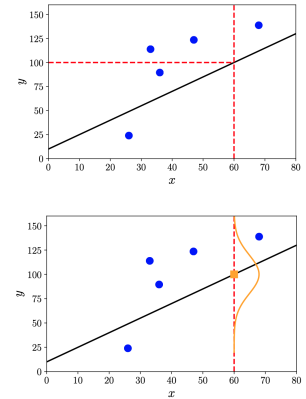
Three algorithmic phases

(1) Prediction or inference: via function or probabilitic models

(2) Training or parameters estimation
  - fixed parameter assumption (non-probabilistic) or Bayesisan approach (probabilistic)
  - non-probabilistic: e.g., empirical risk minimization
  - probabilistic: e.g., ML (Maximum Likelihood), MAP (Maximum A Posteriori)
  - cross-validation: simulation of performing for unseen data
  - regularization/prior: balancing models between training and unseen data

(3) Hyperparameter tuning or model selection

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- Predictor as a function

- Given $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$, estimate a predictor $f(\cdot, \boldsymbol{\theta}) : \mathbb{R}^D \mapsto \mathbb{R}$

- Find a good parameter $\boldsymbol{\theta}^*$, such that $f(\boldsymbol{x}_n, \boldsymbol{\theta}^*) = \hat{y}_n \approx y_n$, for all $n = 1, \ldots, N$

- Example. Affine function: By adding the unit feature $x^{(0)} = 1$ and θ_0, i.e.,
$$\boldsymbol{x}_n = [1, x_n^{(1)}, \ldots, x_n^{(D)}]^\top, \; \boldsymbol{\theta} = [\theta_0, \theta_1, \ldots, \theta_D]^\top$$
$$f(\boldsymbol{x}_n, \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{x}_n = \theta_0 + \sum_{d=1}^{D} \theta_d x_n^{(d)}$$

- Example. Neural network: Complex non-linear function

- Training set: $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n), \ldots, (\boldsymbol{x}_N, y_N)\}$, an example matrix[1] $\boldsymbol{X} := [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N]^\top \in \mathbb{R}^{N \times D}$, a label vector $\boldsymbol{y} := [y_1, \ldots, y_N]^\top$,

- Average loss, empirical risk
$$\boldsymbol{R}_{\text{emp}}(f, \boldsymbol{X}, \boldsymbol{y}) = \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, \hat{y}_n)$$

- 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) $\boldsymbol{R}_{\text{true}} = \mathbb{E}_{\boldsymbol{x}, y}[\ell(y, f(\boldsymbol{x}))]$?

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[1]In other chapters, we often use $D \times N$ example matrix by defining it as $\boldsymbol{X} := [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N]$. L10(4)

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

  ◦ $\|\boldsymbol{\theta}\|^2$: regularizer, λ: regularization parameter
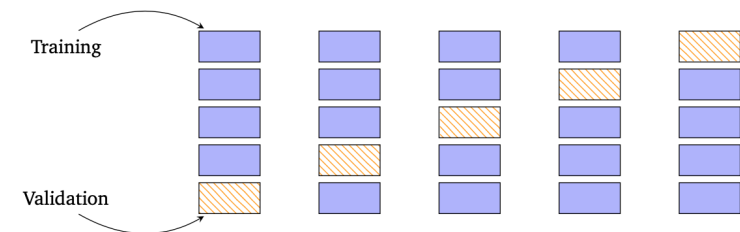
- Idea: define a function of the parameters called likelihood function.
- Negative log-likelihood for data $\boldsymbol{x}$ and a family of probability densities $\mathbb{P}(\boldsymbol{x} \mid \boldsymbol{\theta})$ parameterized by $\boldsymbol{\theta}$:

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

  ○ $\mathcal{L}(\boldsymbol{\theta})$: how likely a particular setting of $\boldsymbol{\theta}$ is for the observations $\boldsymbol{x}$.

- MLE: Find $\boldsymbol{\theta}$ such that $\mathcal{L}(\boldsymbol{\theta})$ is minimized (i.e., likelihood is maximized)

- The set of iid examples $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)$
- $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ and $\mathcal{Y} = \{y_1, \ldots, y_N\}$
- Negative log-likelihood

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

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

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

- What if we have some prior knowledge about $\boldsymbol{\theta}$? Then, how should we change our knowledge about $\boldsymbol{\theta}$ after observing data $\boldsymbol{x}$?
- Compute a posteriori distribution (using Bayes' Theorem) and find $\boldsymbol{\theta}$ that maximizes the distribution:
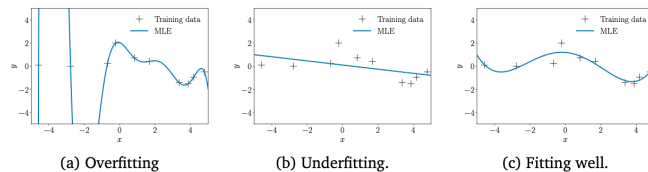
$$\max_{\boldsymbol{\theta}} \mathbb{P}(\boldsymbol{\theta} \mid \boldsymbol{x}) = \max_{\boldsymbol{\theta}} \frac{\mathbb{P}(\boldsymbol{x} \mid \boldsymbol{\theta}) \mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\boldsymbol{x})} \iff \min_{\boldsymbol{\theta}} \left(-\log \mathbb{P}(\boldsymbol{\theta} \mid \boldsymbol{x})\right)$$

  ○ In finding the optimal $\boldsymbol{\theta}$, $\mathbb{P}(\boldsymbol{x})$ 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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- Model class $M_{\boldsymbol{\theta}}$ vs. Right model M^*
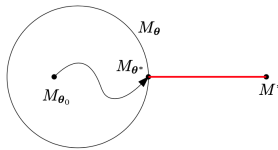
- Overfitting vs. Underfitting vs. Good fitting

(a) Overfitting   (b) Underfitting.   (c) Fitting well.

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Roadmap

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Modeling Generative Process and Probabilistic Models

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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 $\mathbb{P}(\boldsymbol{x}, \boldsymbol{\theta})$ of the observed variables $\boldsymbol{x}$ and the hidden parameters $\boldsymbol{\theta}$ encapsulate the key information
  - Given: prior $\mathbb{P}(\boldsymbol{\theta})$ and likelihood $\mathbb{P}(\boldsymbol{x}|\boldsymbol{\theta})$
  - Joint dist. from prior and likelihood: $\mathbb{P}(\boldsymbol{x}, \boldsymbol{\theta}) = \mathbb{P}(\boldsymbol{x}|\boldsymbol{\theta})\mathbb{P}(\boldsymbol{\theta})$
  - We get: marginal likelihood $\mathbb{P}(\boldsymbol{x}) = \int \mathbb{P}(\boldsymbol{x}, \boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}$ and posterior $\mathbb{P}(\boldsymbol{\theta}|\boldsymbol{x}) = \frac{\mathbb{P}(\boldsymbol{x}, \boldsymbol{\theta})}{\mathbb{P}(\boldsymbol{x})}$

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Fully Bayesian vs. ML/MAP

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

- 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 $\boldsymbol{\theta}$

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

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

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

$$\mathbb{P}(\boldsymbol{\theta} \mid \mathcal{X}) = \frac{\mathbb{P}(\mathcal{X} \mid \boldsymbol{\theta})\mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\mathcal{X})}, \quad \mathbb{P}(\mathcal{X}) = \int \mathbb{P}(\mathcal{X} \mid \boldsymbol{\theta})\mathbb{P}(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}$$

- 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

- Including latent variables in the model $\rightarrow$ contributing to the interpretability of the model

- General discussions here would be applied the following examples later
  - PCA for dimensionality reduction   L10(7)

  - Gaussian mixture models for density estimation   L11(3)

- In latent-variable models (LVMs)[2],
  - Given: prior $\mathbb{P}(\boldsymbol{z})$ and likelihood $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$

  - Joint dist. from prior and likelihood: $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}) = \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\mathbb{P}(\boldsymbol{z})$

  - Our interest: marginal likelihood $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})$ and posterior $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$

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

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

- Inference. computing the posterior distribution $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$:

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

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

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

- Explanation of the observation. Allows us to figure out which latent configurations could have plausibly generated the observation data samples.

- Learning of model parameters $\boldsymbol{\theta}$. Training LVMs to estimate $\boldsymbol{\theta}$ (e.g., ML) requires $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ in its inner loops

> marginal likelihood $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}) \implies$ posterior distribution $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}) \implies \boldsymbol{\theta}_{\mathrm{ML}}$

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

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

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

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Graphical Models   **KAIST EE**   Graph Semantics   **KAIST EE**

- 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
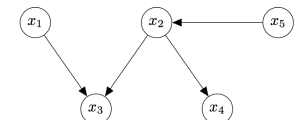
$$\mathbb{P}(a, b, c) = \mathbb{P}(c|a, b)\mathbb{P}(b|a)\mathbb{P}(a)$$
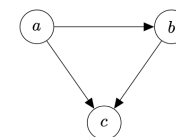
(a) Fully connected.

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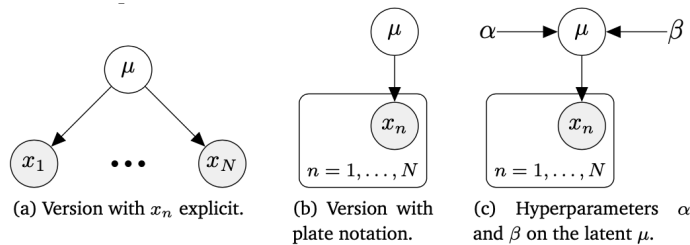

(b) Not fully connected.

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

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

(a) Version with x_n explicit.

(b) Version with plate notation.

(c) Hyperparameters α and β on the latent μ.

- Shaded nodes: observables, μ: probability of head, a (latent) random variable
- Joint distribution

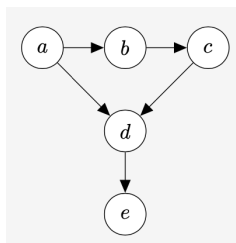$$\mathbb{P}(x_1, \ldots, x_N \mid \mu) = \prod_{n=1}^{N} \mathbb{P}(x_n \mid \mu)$$

- **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
  - All possible trails[3] 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 $\mathcal{C}$
    - ▶ The arrows meet head to head at the node, and neither the node nor any of its descendants is in $\mathcal{C}$
  - If all the paths are blocked, then $\mathcal{A}$ is *d*-separated from $\mathcal{B}$ by $\mathcal{C}$.
  - If *d*-separated, $\mathcal{A} \perp\!\!\!\perp \mathcal{B} \mid \mathcal{C}$

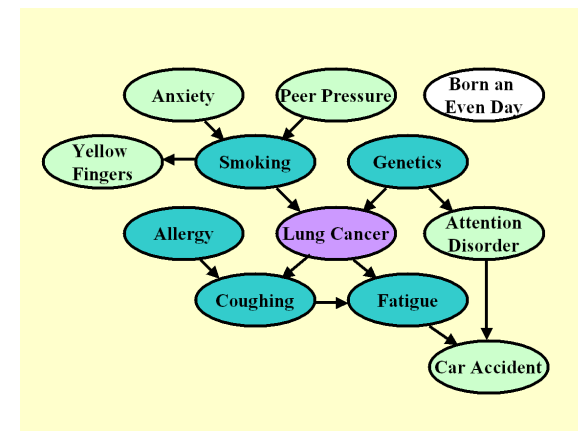[3]paths that ignore the direction of the arrows

- $b \perp\!\!\!\perp d \mid a, c$
- $a \perp\!\!\!\perp c \mid b$
- $b \not\perp\!\!\!\perp d \mid c$
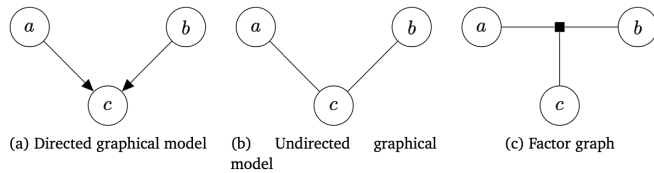- $a \not\perp\!\!\!\perp c \mid b, e$

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

Three Types of Graphical Models

(a) Directed graphical model   (b) Undirected graphical model   (c) Factor graph

- Directed graphical models (or Bayesian Networks)

- Undirected graphical models (Markov Random Fields)

- Factor graphs

Roadmap

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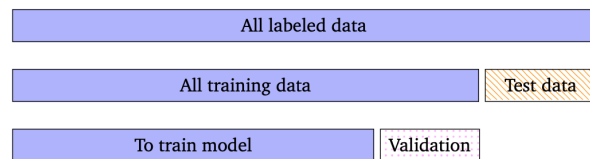
- Model selection
  - Tradeoff between model complexity and data fit
  - Occam's razor. Find the simplest model that explains the data resonably well.
- Test set: estimate the generalization performance
- Validation set: choose the best model

Bayesian Model Selection

- A set of models $\boldsymbol{M} = \{M_1, \ldots, M_k\}$, where each M_k has $\boldsymbol{\theta}_k$ parameters. A prior $\mathbb{P}(M)$ on each model $M \in \boldsymbol{M}$.

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

- 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:

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

- 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:

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

- $\mathbb{P}(\mathcal{D} \mid M_k)$: How well the data is predicted by the model M_k

- 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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1)

Questions?