

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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Roadmap

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

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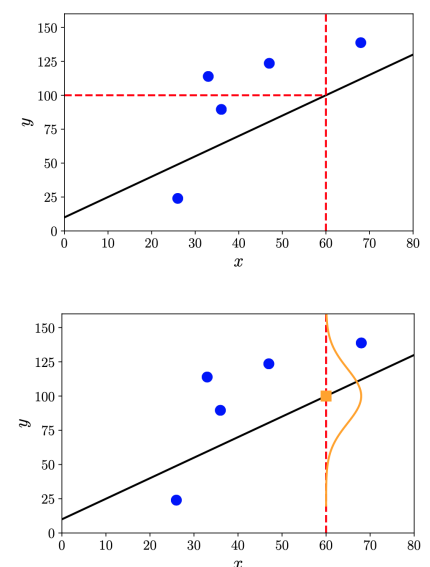
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- Three major components of a machine learning system
 1. Data: $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n), \dots, (\mathbf{x}_N, y_N)\}$
 2. Models: functions or probabilistic models
 3. Learning: Training, and prediction/inference
- Good 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 $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$
- In supervised learning, $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n), \dots, (\mathbf{x}_N, y_N)\}$, 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 (PCA via SVD or EVD)
 - using nonlinear higher-dimensional combinations of the original feature vector (feature map and kernel)

Models: Functions vs. Probabilistic Models

- Now, the business of constructing a predictor.
- Models as **functions**
 - $f : \mathbb{R}^D \mapsto \mathbb{R}$.
 - **Example.** $f(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x} + \theta_0$, 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 (mean and variance of Gaussian)



- Three algorithmic phases
 - (1) Prediction or inference: via function or probabilistic models
 - (2) Training or parameters estimation
 - fixed parameter assumption (non-probabilistic) or Bayesian 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 $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n), \dots, (\mathbf{x}_N, y_N)\}$, estimate a predictor $f(\cdot, \boldsymbol{\theta}) : \mathbb{R}^D \mapsto \mathbb{R}$
- Find a good parameter $\boldsymbol{\theta}^*$, such that $f(\mathbf{x}_n, \boldsymbol{\theta}^*) = \hat{y}_n \approx y_n$, for all $n = 1, \dots, N$
- **Example.** Affine function: By adding the unit feature $x^{(0)} = 1$ and θ_0 , i.e.,
 $\mathbf{x}_n = [1, x_n^{(1)}, \dots, x_n^{(D)}]^\top$, $\boldsymbol{\theta} = [\theta_0, \theta_1, \dots, \theta_D]^\top$

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

- **Example.** Neural network: Complex non-linear function

Loss Function

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

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

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

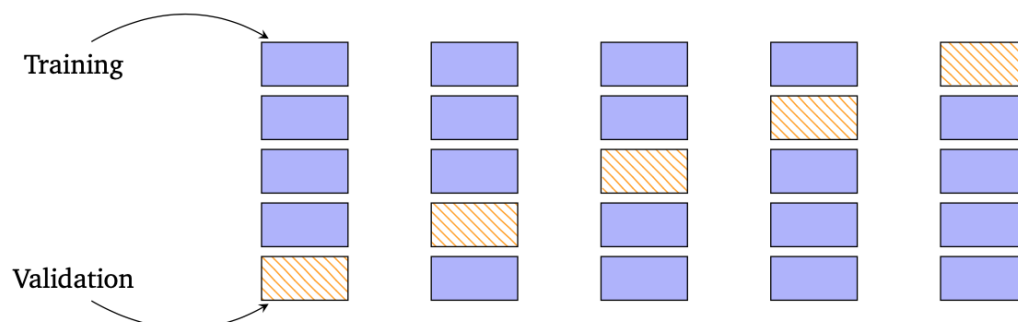
$$\min_{\boldsymbol{\theta} \in \mathbb{R}^D} \frac{1}{N} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|^2$$

- **Question.** Ultimate goal: Minimizing expected risk (for unseen data)
 $R_{\text{true}} = \mathbb{E}_{\mathbf{x}, y}[\ell(y, f(\mathbf{x}))]$?

- 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

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

- $\|\theta\|^2$: regularizer, λ : regularization parameter



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MLE (Maximum Likelihood Estimation): Concepts

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

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

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

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

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

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

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

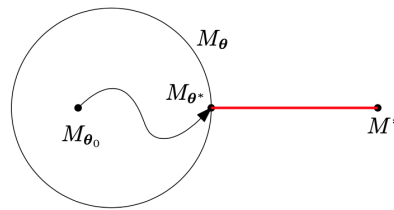
MAP (Maximum A Posteriori)

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

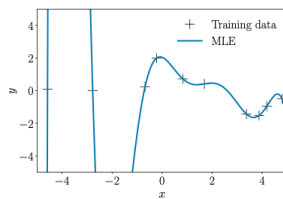
$$\max_{\boldsymbol{\theta}} \mathbb{P}(\boldsymbol{\theta} \mid \mathbf{x}) = \max_{\boldsymbol{\theta}} \frac{\mathbb{P}(\mathbf{x} \mid \boldsymbol{\theta}) \mathbb{P}(\boldsymbol{\theta})}{\mathbb{P}(\mathbf{x})} \iff \min_{\boldsymbol{\theta}} \left(-\log \mathbb{P}(\boldsymbol{\theta} \mid \mathbf{x}) \right)$$

- In finding the optimal $\boldsymbol{\theta}$, $\mathbb{P}(\mathbf{x})$ 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).
- We later see the full parameter distributions

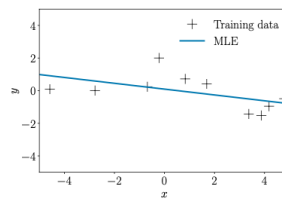
- Model class M_θ vs. Right model M^*



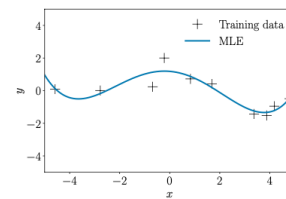
- Overfitting vs. Underfitting vs. Good fitting



(a) Overfitting



(b) Underfitting.



(c) Fitting well.

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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 $\mathbb{P}(\mathbf{x}, \boldsymbol{\theta})$ of the observed variables \mathbf{x} and the hidden parameters $\boldsymbol{\theta}$ encapsulate the key information
 - the prior and likelihood, marginal distribution, and the posterior
- Essentially, if we know the joint distribution, we know all about its probabilistic model

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Bayesian Inference

- Earlier, two ways of estimating the parameter $\boldsymbol{\theta}$: ML and MAP. Essentially, it is solving an optimization problem to get a single best value $\boldsymbol{\theta}^*$. \implies Prediction through $\mathbb{P}(\mathbf{x} \mid \boldsymbol{\theta}^*)$.
- Rather than just a likelihood, having the full posterior distribution can be useful. For a data set \mathcal{X} , a parameter prior $\mathbb{P}(\boldsymbol{\theta})$, and a likelihood function, the posterior is:

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

- **Question.** Examples of prediction using the posterior distribution?
- Bayesian inference requires to solving 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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Given the data set \mathcal{X} , we want to predict A , we want to do the following prediction:

$$\mathbb{P}(A | \mathcal{X})$$

- **ML**: Easy (high), Exact (low)

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

- **MAP**: Easy (mid), Exact (mid)

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

- **Fully Bayesian**: Easy (low), Exact (high)

- predictive inference, use of posterior predictive distribution, bayesian prediction

$$\mathbb{P}(A | \mathcal{X}) = \int \mathbb{P}(A | \theta) \mathbb{P}(\theta | \mathcal{X}) d\theta$$

- Including latent variables in the model: Contributing to the interpretability of the model
- Examples: PCA for dimensionality reduction, Gaussian mixture models for density estimation
- Offers data generation process through parameters: $\mathbb{P}(\mathbf{x} | \theta, \mathbf{z})$, $\mathbb{P}(\mathbf{z})$
- Marginalization over the latent variables, which allows parameter estimation by ML and MAP (using the prior $\mathbb{P}(\theta)$)

$$\mathbb{P}(\mathbf{x} | \theta) = \int \mathbb{P}(\mathbf{x} | \theta, \mathbf{z}) \mathbb{P}(\mathbf{z}) d\mathbf{z}$$

- We can compute a posterior on the latent variables, but marginalizing over both \mathbf{z} and θ is hard:

$$\mathbb{P}(\mathbf{z} | \mathcal{X}) = \frac{\mathbb{P}(\mathcal{X} | \mathbf{z}) \mathbb{P}(\mathbf{z})}{\mathbb{P}(\mathcal{X})}, \quad \mathbb{P}(\mathcal{X} | \mathbf{z}) = \int \mathbb{P}(\mathcal{X} | \mathbf{z}, \theta) \mathbb{P}(\theta) d\theta$$

- Instead, it is easier to compute the latent-variable posterior, but conditioned on the model parameters, i.e.,

$$\mathbb{P}(\mathbf{z} \mid \mathcal{X}, \boldsymbol{\theta}) = \frac{\mathbb{P}(\mathcal{X} \mid \mathbf{z}, \boldsymbol{\theta})\mathbb{P}(\mathbf{z})}{\mathbb{P}(\mathcal{X} \mid \boldsymbol{\theta})}$$

- **Question.** How do we use the posteriors $\mathbb{P}(\mathbf{z} \mid \mathcal{X})$ or $\mathbb{P}(\mathbf{z} \mid \mathcal{X}, \boldsymbol{\theta})$ in practice? Any examples?

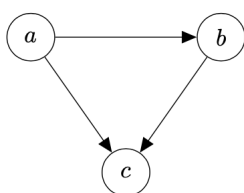
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- Joint distribution of a probabilistic model: key quantity of interest, but quite complicated without structural properties
- However, there exist relations of **independence**, **conditional independence** among random variables.
- (Probabilistic) 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

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Graph Semantics

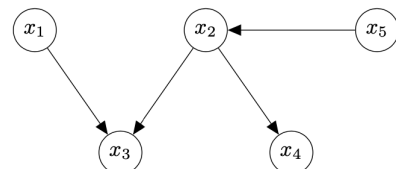
$$\mathbb{P}(a, b, c) = \mathbb{P}(c|a, b)\mathbb{P}(b|a)\mathbb{P}(a)$$



(a) Fully connected.

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

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

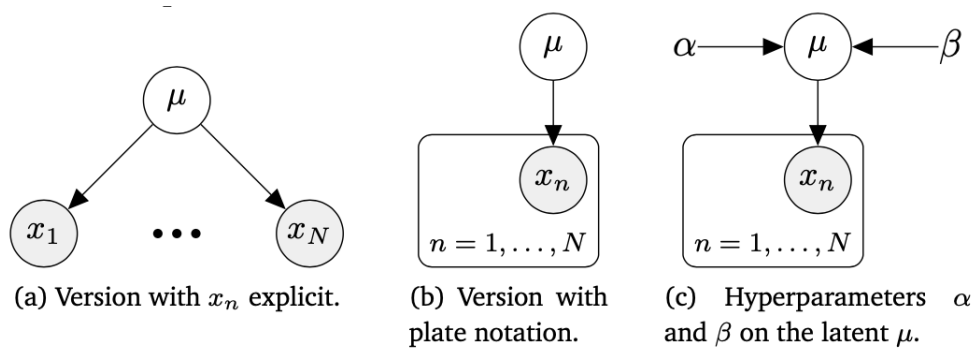


(b) Not fully connected.

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

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

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

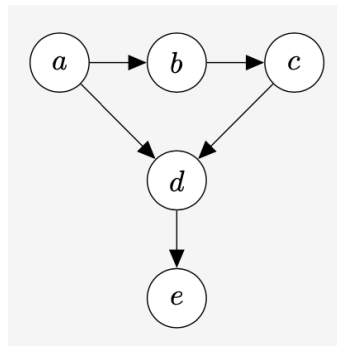
$$\mathbb{P}(x_1, \dots, x_N \mid \mu) = \prod_{n=1}^N \mathbb{P}(x_n \mid \mu)$$

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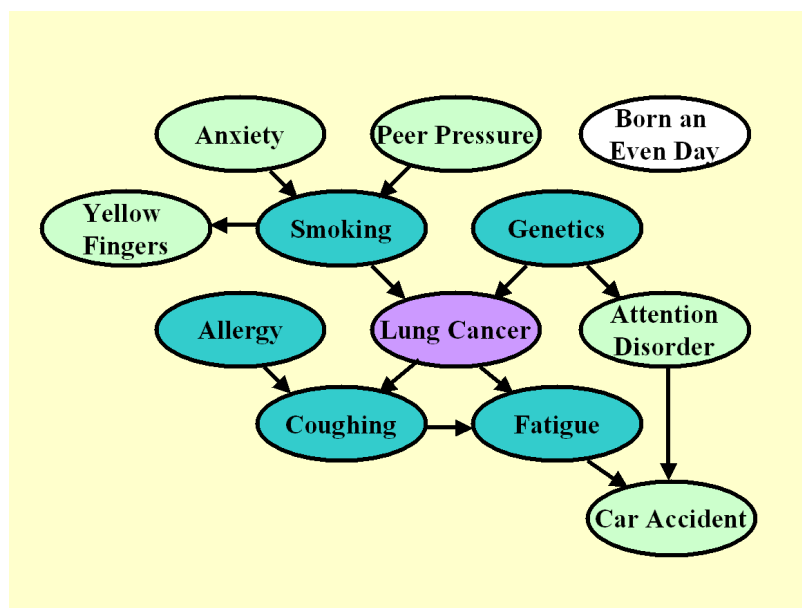
Conditional Independence and d -Separation

- **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 trails¹ 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, $\mathcal{A} \perp\!\!\!\perp \mathcal{B} \mid \mathcal{C}$

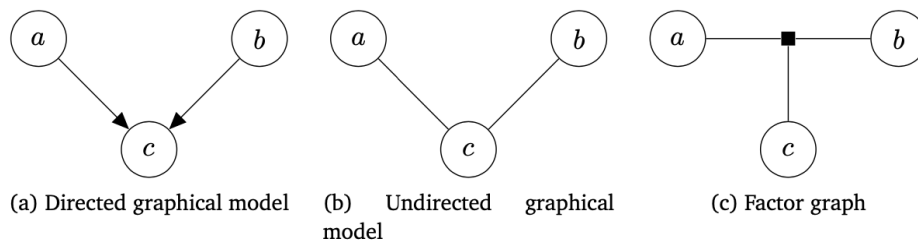
¹paths that ignore the direction of the arrows



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

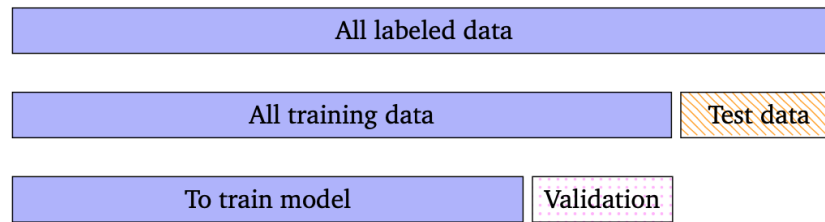


Source: <http://www.causality.inf.ethz.ch/data/LUCAS.html>



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

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- Model selection
 - Tradeoff between model complexity and data fit
 - [Occam's razor](#). Find the simplest model that explains the data reasonably 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 θ_k parameters. A prior $\mathbb{P}(M)$ on each model $M \in \mathbf{M}$.
- Posterior distribution $\mathbb{P}(M_k | \mathcal{D}) \propto \mathbb{P}(M_k) \mathbb{P}(\mathcal{D} | M_k)$, where we have the following [model evidence](#) or [marginal likelihood](#):

$$\mathbb{P}(\mathcal{D} | M_k) = \int \mathbb{P}(\mathcal{D} | \theta_k) \mathbb{P}(\theta_k | M_k) d\theta_k \quad (***)$$

- MAP for the model: $M^* = \arg \max_{M_k} \mathbb{P}(M_k | \mathcal{D})$
- 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 :

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

- $\mathbb{P}(\mathcal{D} | M_k)$: 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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Questions?

Review Questions

1)