Structure learning and the generalization capacity of algorithms

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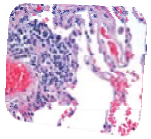
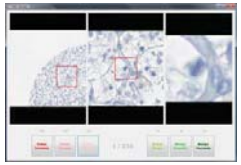
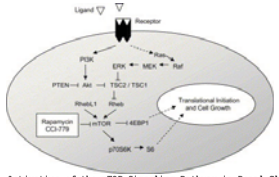
Modern information society and the Information Technology value chain

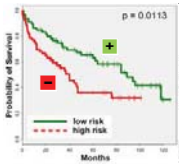






Activation of the mTOR Signaling Pathway in Renal Clear Cell Carcinoma. Robb et al., J Urology 177:346 (2007)

Data → **Information** → **Knowledge** → **Value**



Unsolved Problems in Computer Science:

1) What is useful information?

2) How can we design robust algorithms?

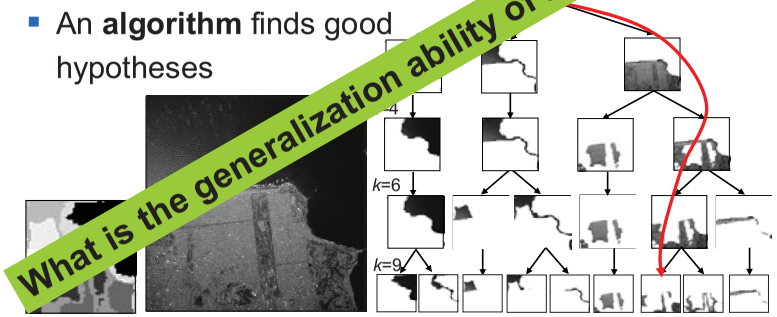
*my**Vision***: **Information theory** for **pattern analysis**

- **Approximation capacity** of algorithms
- Examples for cost function minimization
  - Cluster validation
  - Role based access control
  - (Robust SVD)
- Philosophical remarks

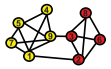
Pattern recognition and modeling

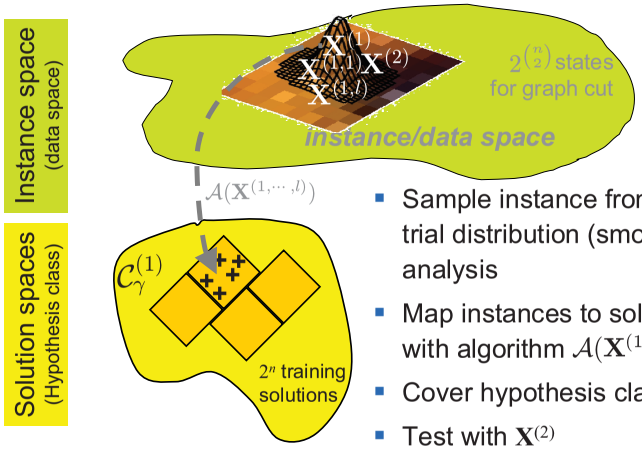
- Given are **data** $\mathbf{X}$ and **hypotheses**, i.e. interpretation of these data.
- An **algorithm** finds good hypotheses

What is the generalization ability of an algorithm?



Generalization of algorithms

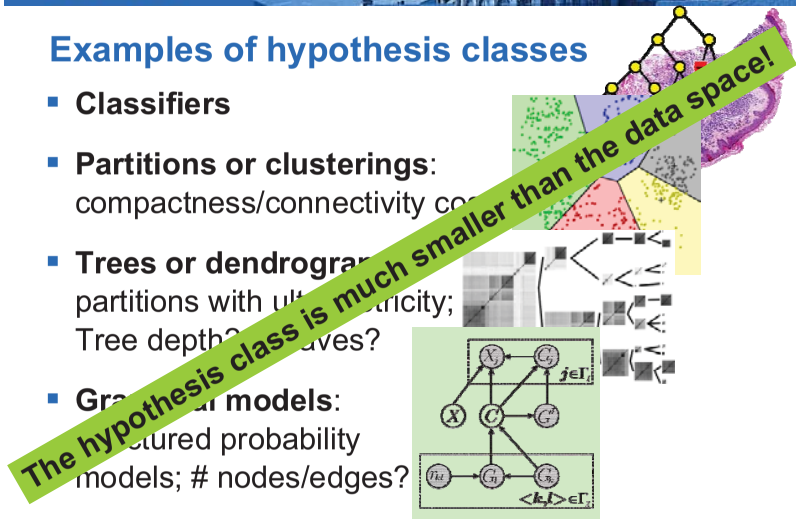




- Sample instance from a trial distribution (smoothed analysis
- Map instances to solutions with algorithm $\mathcal{A}(\mathbf{X}^{(1,\cdots,l)})$
- Cover hypothesis class
- Test with $\mathbf{X}^{(2)}$

Examples of hypothesis classes

- **Classifiers**
- **Partitions or clusterings**: compactness/connectivity co
- **Trees or dendrogra** partitions with ul tricity; Tree depth? aves?
- **Gra al models**: tured probability models; # nodes/edges?

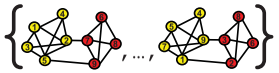


Information Theory & Pattern Recognition

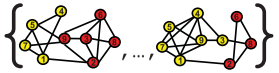
- IT-Components
  - **Code book** $\subsetneq$ **{strings}** = hypothesis class

0000000	0100101	1000011	1100110
0001111	0101010	1001100	1101001
0010110	0110011	1010101	1110000
0011001	0111100	1011010	1111111

  - Noisy **channel**
    1100110 -> 0110110
  - Decoder: minimize **Hamming distance**
    |0110110−1100110| <
    |0110110−1010101|
- Pattern Recognition elements
  - **Set of approximation sets** $\subsetneq$ **hypothesis class**



  - Noisy **optimization** problem



  - Decoding by **approximate optimization** of test instance

Symmetries of the Learning Problem

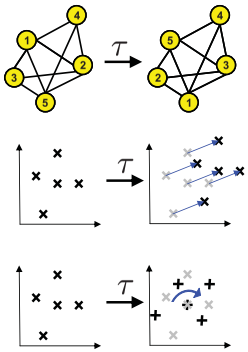
- Assume (!) that the algorithm $\mathcal{A}$ is equivariant under the transformations

$$\mathcal{T} = \{\tau : \tau \circ \mathcal{A}(\mathbf{X}) = \mathcal{A}(\tau_{\mathbf{X}} \circ \mathbf{X})\}$$

- **Idea**: define a code by transforming a given problem => codebook $\mathbb{T} = \{\tau_i \in \mathcal{T} : 1 \leq i \leq 2^{n\rho}\}$
- What is an appropriate set of transformations? That depends on the algorithm and the hypothesis class!

How to generate code problems?

1. Combinatorial optimization problems: **permutation** of e.g. vertices in graphs
2. Localization problems: **shifts** of data
3. Orientation problems (PCA, SVD): **rotations & projection**
4. Sparse linear regression: **Scaling & permutation**



Approximate Optimization

- Define weights for hypotheses with low costs

$$w_\beta(c, \mathbf{X}) = \exp(-\beta R(c, \mathbf{X})) \quad c \in \mathcal{C}(\mathbf{X})$$

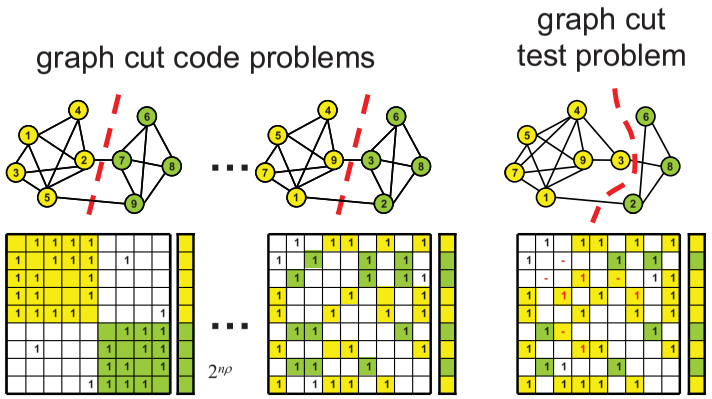
- Special case: **Approximation set**

$$w_\beta(c, \mathbf{X}) = \begin{cases} 1, & R(c, \mathbf{X}) \leq R\left(c^\perp, \mathbf{X}\right) + \gamma; \\ 0, & \text{otherwise.} \end{cases}$$

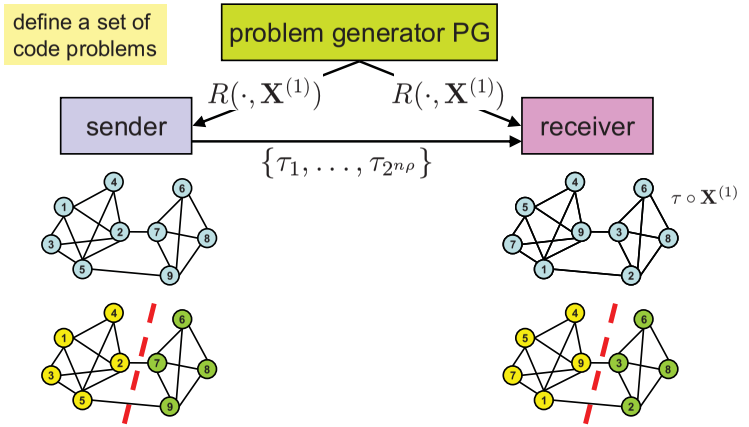
- Total weight of low cost hypotheses

$$W_\beta(\mathbf{X}) = \{w_\beta(c, \mathbf{X}) : c \in \mathcal{C}(\mathbf{X})\}$$

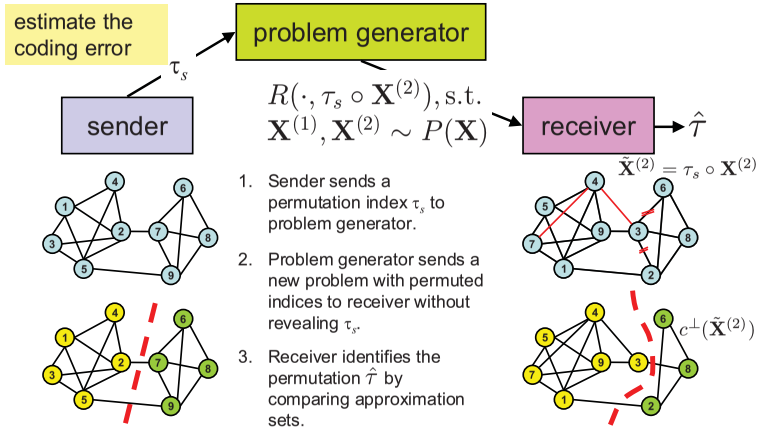
Code problem generation for Graph Cut



Coding with Graph Cut approximation sets



Communication by approximation sets



1. Sender sends a permutation index τ_s to problem generator.
2. Problem generator sends a new problem with permuted indices to receiver without revealing τ_s.
3. Receiver identifies the permutation $\hat{\tau}$ by comparing approximation sets.

Communication Process

- Receiver **compares sets of hypothesis weights** $W_\beta(\mathbf{X}^{(1)})$ of training instance (code problem) with approximate clusterings $W_\beta(\mathbf{X}^{(2)})$ of the test data.
- Define a mapping $\psi : \mathbf{X}^{(1)} \to \mathbf{X}^{(2)}$
- **Decoding by maximizing weight overlap**

$$\hat{\tau} \in \arg\max_{\tau \in \mathbb{T}} \sum_{c \in \mathcal{C}(\mathbf{X}^{(1)})} w_\beta\left(c, \tau(\mathbf{X}^{(1)})\right) w_\beta\left(c, \tilde{\mathbf{X}}^{(2)}\right)$$

$$\text{with } \tilde{\mathbf{X}}^{(2)} := \psi \circ \tau_s \circ \psi^{-1}(\mathbf{X}^{(2)})$$

Condition of vanishing total error

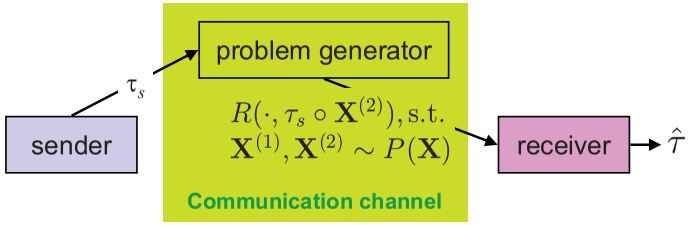
$\lim_{n\to\infty} P(\hat{\tau} \neq \tau_s | \tau_s) = 0$ yields

- Rate is bounded by mutual information

$$\begin{aligned} \rho \log 2 &< \frac{1}{n} \log \frac{|\{\tau_{\neq s}\}| Z_{\beta,s}^{(1\&2)}}{Z_\beta^{(1)} Z_\beta^{(2)}} \\ &= \frac{1}{n}\left(\log \frac{|\{\tau_{\neq s}\}|}{Z_\beta^{(1)}} + \log \frac{|\mathcal{C}^{(2)}|}{Z_\beta^{(2)}} - \log \frac{|\mathcal{C}^{(2)}|}{Z_{\beta,s}^{(1\&2)}}\right) \\ &\equiv \mathcal{I}_\gamma(\tau_s, \hat{\tau}) \end{aligned}$$

- Lower bound: generalize Fano's inequality to ASC (work in progress)

Model Selection by Maximization of Approximation Capacity

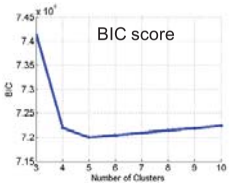


- Optimize the communication channel w.r.t. approximation quality γ (β), topology and metric of solution space, cost function $R(.,.)$, transfer function ψ

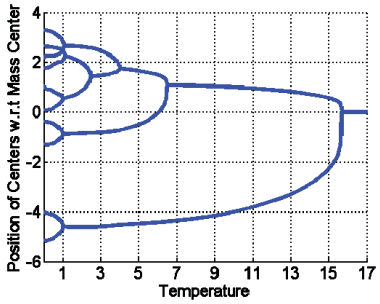
2d Mixture Model Estimation

Experimental Setting:

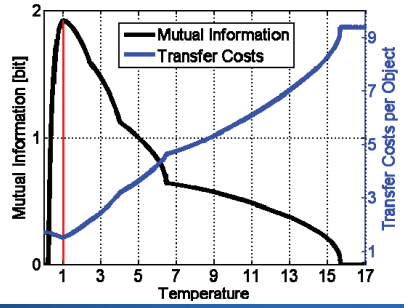
5 Gaussians, n=10000, d=2, k^{max}=10



Cluster splitting



Approximation Capacity



Conclusion

- **Quantization**: Noise quantizes mathematical structures (hypothesis classes) **=>** symbols
- These symbols can be used for **coding**!
- Optimal error free coding scheme determines **approximation capacity** of a model class.

⇒Bounds for robust optimization.

⇒**Quantization** of hypothesis class measures **structure specific information** in data.

Future Work

- **Generalization**: replace approximation sets based on cost functions by smoothed outputs of **algorithms** ("smoothed generalization")
- **Model reduction** in dynamical systems: quantize sets of ODEs or PDEs (systems biology)
- Relate **statistical complexity**, i.e. the approximation capacity, to algorithmic or **computational complexity**.

Philosophical speculations

- We experience a **paradigm shift from model driven reasoning to algorithm dominated reasoning** (Bernard Chazelle "The Algorithm: Idiom of Modern Science")

=> model validation more essential than modeling since modeling can be algorithmically formulated as exploration of model space.

- *Ceterum censeo*: The coupling of **statistical complexity** and **algorithmic complexity** should be reconsidered in the light of **statistical learning theory** and information theory.