ETH
Eidgenössische Technische Hochschule Zürich
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inf | Informatik
Computer Science

Information theory of algorithms

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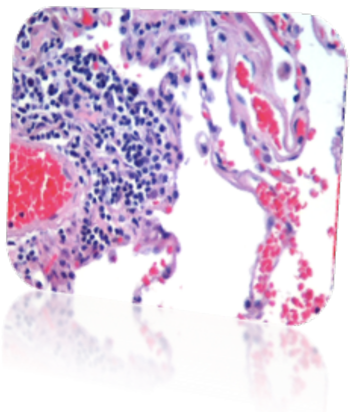
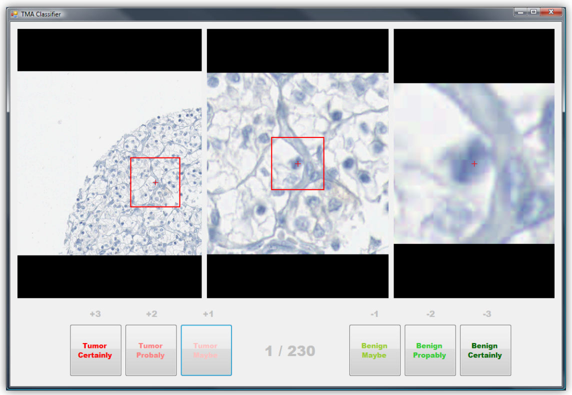
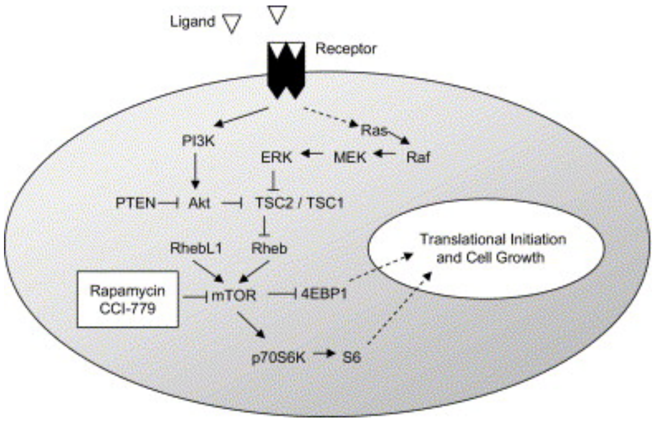
IT value for personalized medicine

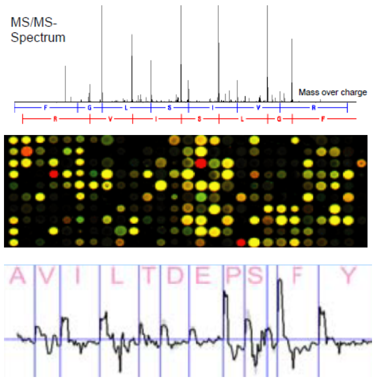


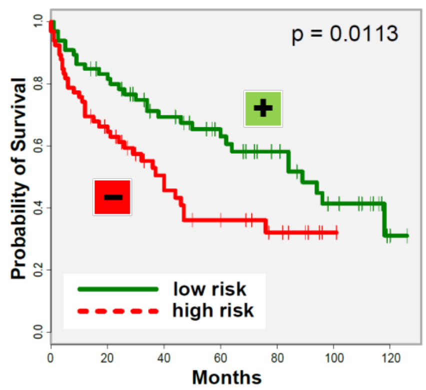




Activation of the mTOR Signaling Pathway in Renal Clear Cell Carcinoma. Robb et al., J Urology 177:346 (2007)

my **Data** → *my* **Information** → *my* **Knowledge**





my **Value**

Roadmap

- **Robust computation versus learning**
  Measuring the information content of algorithms
- **Algorithm/Model validation** by information theory
- **Learning optimal algorithms**: open challenge!
  - Validating approximate spanning trees
  - Graph cut for gene expression analysis
  - Robust sorting

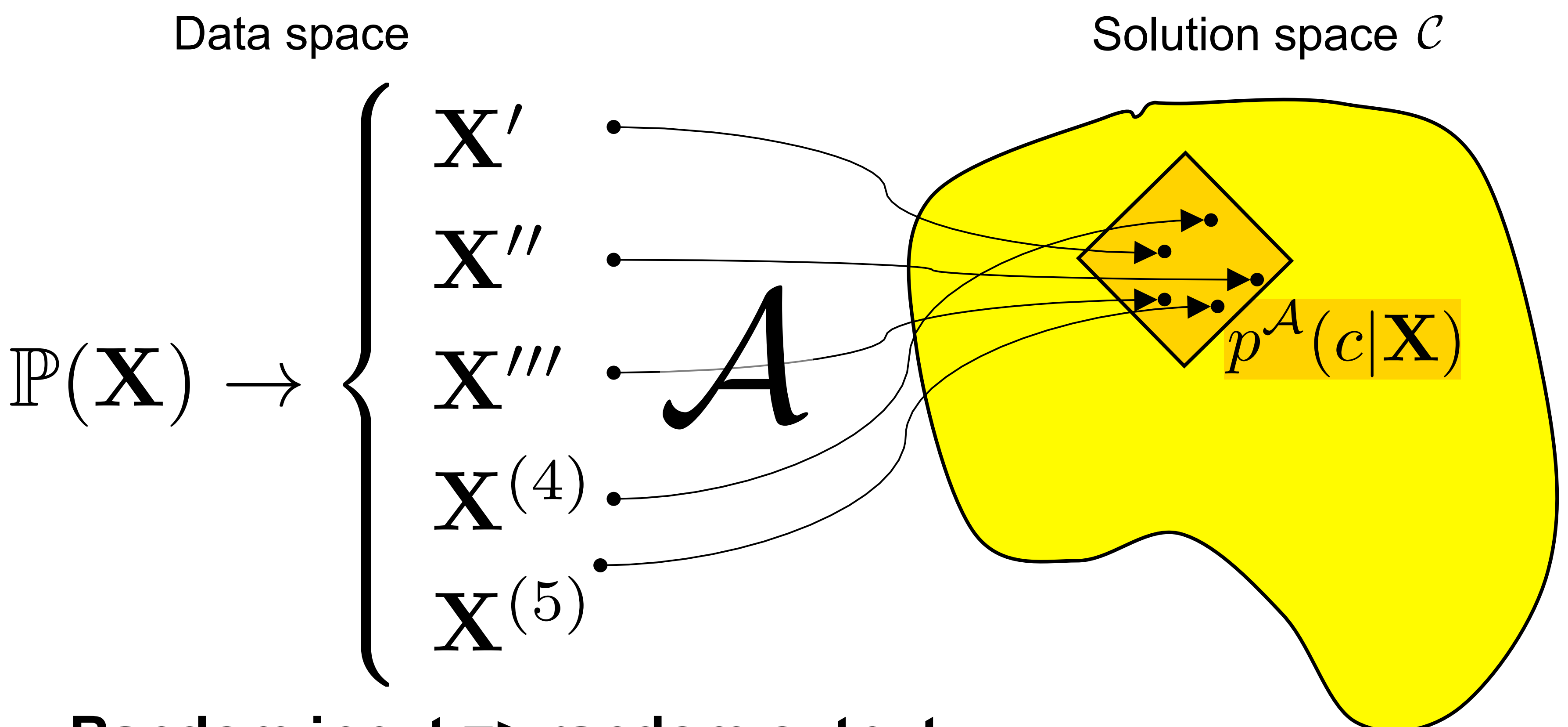
What is an algorithms?

- Informally, an **algorithm** is any well-defined computational procedure that takes some value(s) as **input** and produces some value(s) as **output** (CLRS' 01)
- **Classical view**: algorithm $\mathcal{A}$ maps (stochastic) data (input) to a solution / hypothesis (output).

$$\text{input } \mathbf{X} \to \mathcal{A} \to \text{output } c \in \mathcal{C}$$

Challenge of robust algorithm design

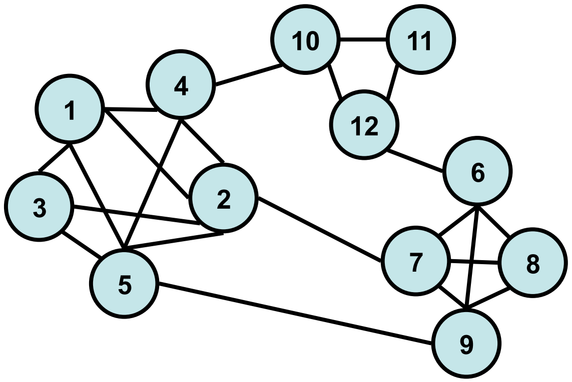
Algorithmic processing: $\text{input } \mathbf{X} \to \mathcal{A} \to \text{output } c \in \mathcal{C}$

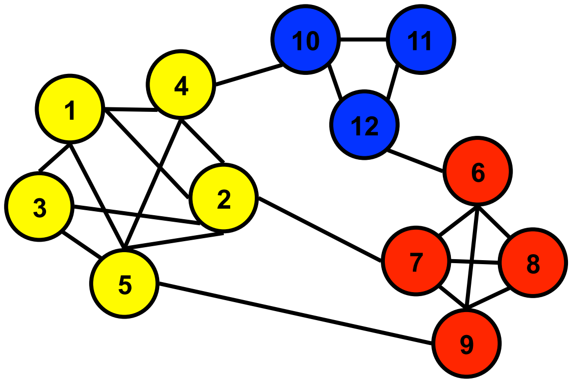


Random input => random output

Core problem in discriminative learning?

- Often, the data space is much larger than the solution space





Space of graphs $\mathfrak{G}_n = \{(\mathcal{V}, \mathcal{E}, \mathcal{W})\}$ with n vertices

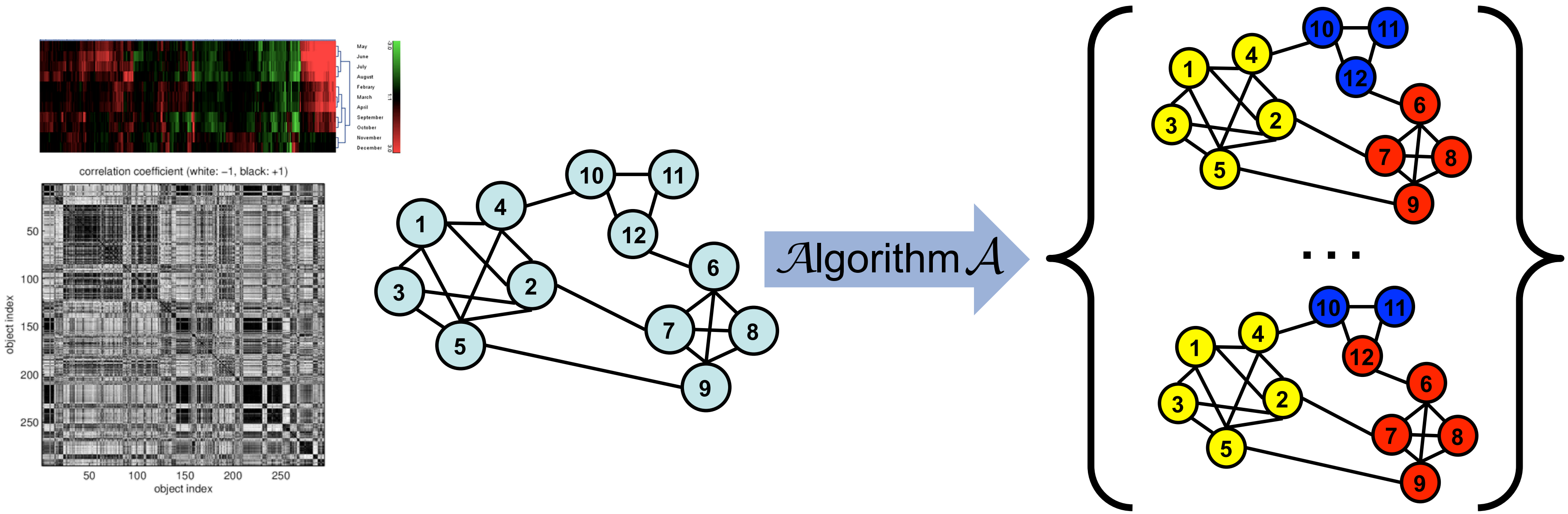
$$|\mathfrak{G}_n| = \mathbb{R}^{\binom{n}{2}}$$

Space of k colorings $\mathcal{C}$

$$|\mathcal{C}| \leq k^n$$

What is learning?

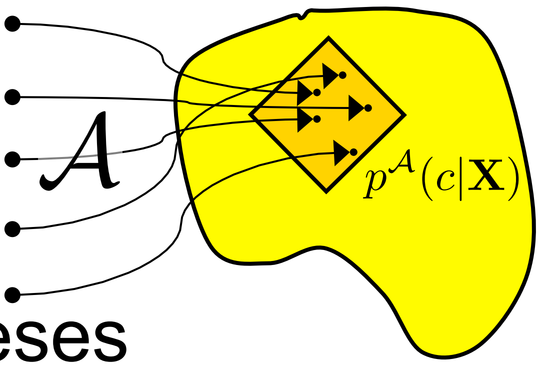
- **Given**: data $\mathbf{X} \sim \mathbb{P}(\mathbf{X})$ and a hypothesis class $\mathcal{C}$



- **Modeling in data analysis** requires
  - **quantization**: given $\mathcal{A}$, identify a set of *good* hypotheses;
  - **learning**: find an $\mathcal{A}$ that specifies an informative set!

Robust algorithms

- For **stochastic input**, an algorithm $\mathcal{A}$ returns a **stochastic output**; we interpret $\mathcal{A}$ as a trajectory in the powerset of the solution space $\mathcal{C}$.



- **Discriminative probabilistic view**: algorithm $\mathcal{A}$ maps stochastic data (input) to a set of solutions / hypotheses $A_t(\mathbf{X})$ (output) still considered at time t
  input $(\mathbf{X}, t^*) \to \mathcal{A} \to$ output posterior $p^{\mathcal{A}}(c|\mathbf{X})$

Algorithms as sets of feasible solutions

- Let X denote data and $A_t(\mathbf{X})$ the set of feasible solutions at iteration t

$$
\begin{aligned}
\text{algorithm } \mathcal{A}(\mathbf{X}) &= \langle A_0(\mathbf{X}), \ldots, A_T(\mathbf{X}) \rangle, \\
\mathbf{init}\ \ A_0(\mathbf{X}) &= \mathcal{C}, \\
A_t(\mathbf{X}) &\subseteq \mathcal{C}, \quad 0 \le t \le T, \\
\mathbf{return}\ \ A_T(\mathbf{X}) &= \{c^\perp(\mathbf{X})\}.
\end{aligned}
$$

- Monotonically contractive algorithms

$$\mathcal{A}(\mathbf{X}) = \langle A_0(\mathbf{X}) \supseteq \ldots \supseteq A_{t^*}(\mathbf{X}) \supseteq \ldots \supseteq A_T(\mathbf{X}) \rangle$$

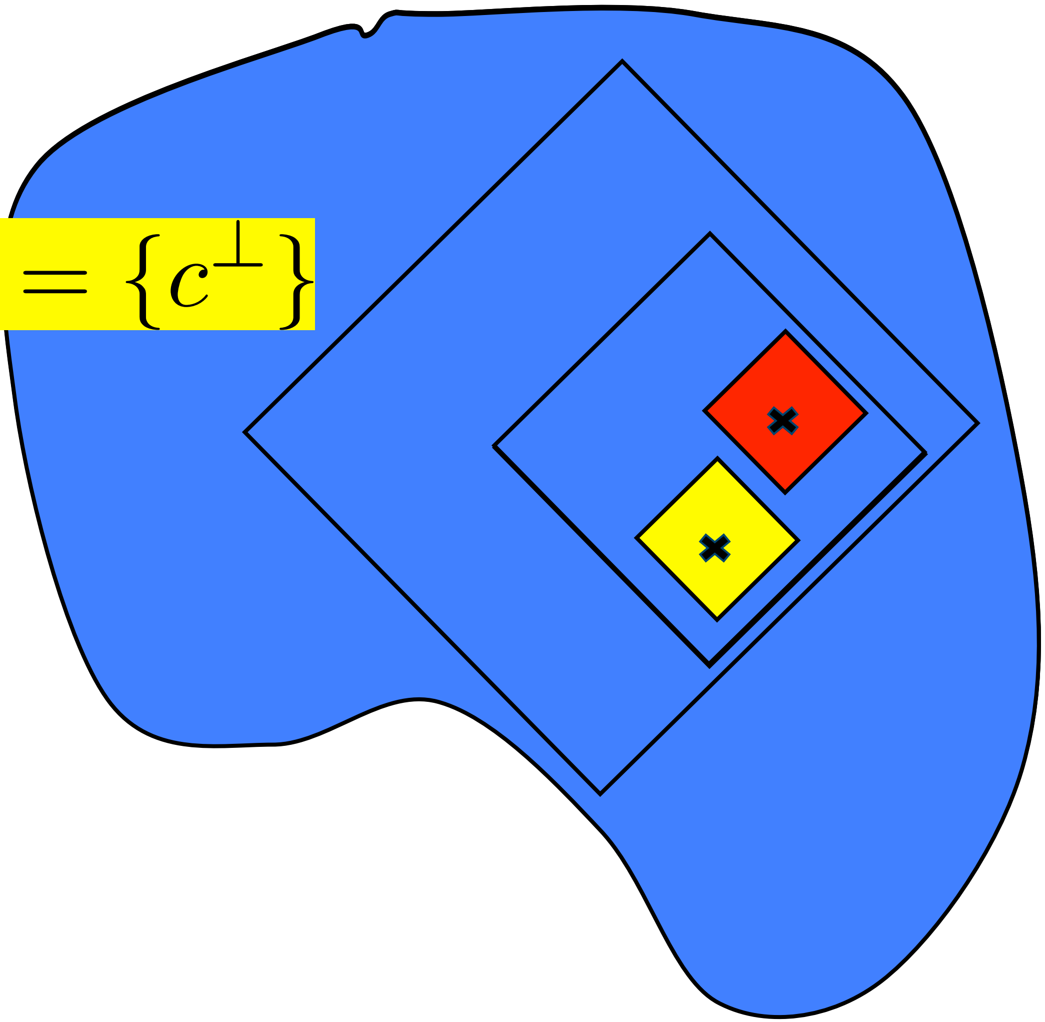
Hypotheses explored by an algorithm $\mathcal{A}$

data $\mathbf{X}'$

data $\mathbf{X}''$

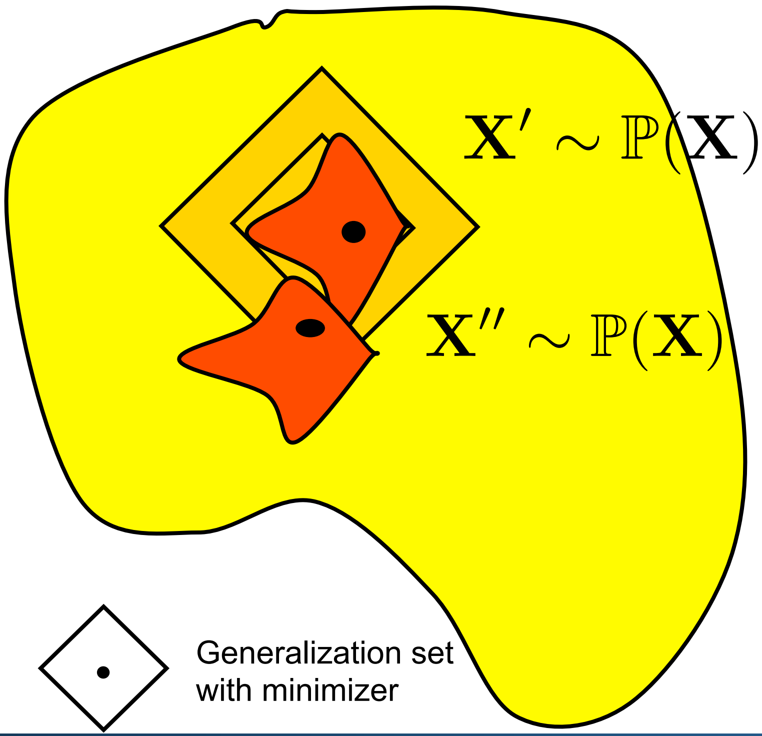
$A_T(\mathbf{X}') = \{c^\perp\}$

$A_T(\mathbf{X}'')$



Coarsening of hypothesis classes and the two instances test

- Quantize **hypothesis class** by generalization sets



- Size: "partition function" at iteration t is $|A_t(\mathbf{X}')|$
- Weight overlap models joint approximations $|A_t(\mathbf{X}') \cap A_t(\mathbf{X}'')|$
- Posterior of hypothesis c

$$p^{\mathcal{A}}(c|\mathbf{X}') = \begin{cases} \dfrac{1}{|A_t(\mathbf{X}')|} & \text{if } c \in A_t(\mathbf{X}') \\ 0 & \text{otherwise} \end{cases}$$

Information theory: structures as symbols

1) sample a hypothesis $\tilde{c} \sim p^{\mathcal{A}}(c|\mathbf{X})$

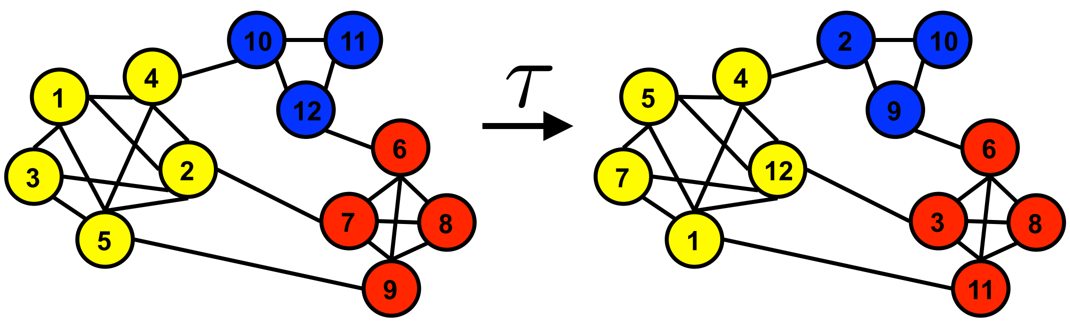
2) for $j = 1 \ldots M$

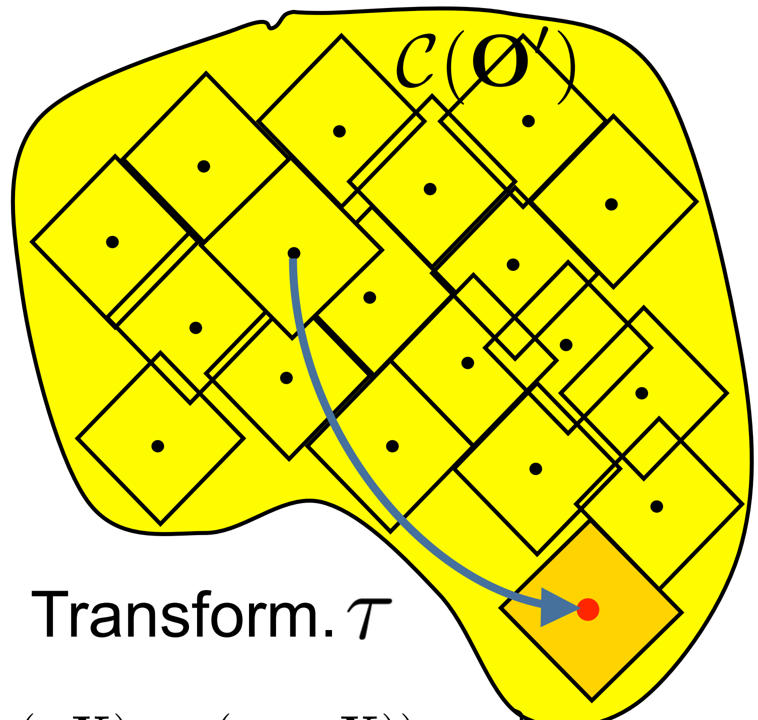
Select a random transf. $\tau_j \in \mathbb{T}(\tilde{c})$

define code vector $\tilde{c}_j := \tau_j \circ \tilde{c}$

3) return codebook $\mathcal{T} := \{\tilde{c}_1, \ldots, \tilde{c}_M\}$

Cover **hypothesis class** densely, but identifiably!



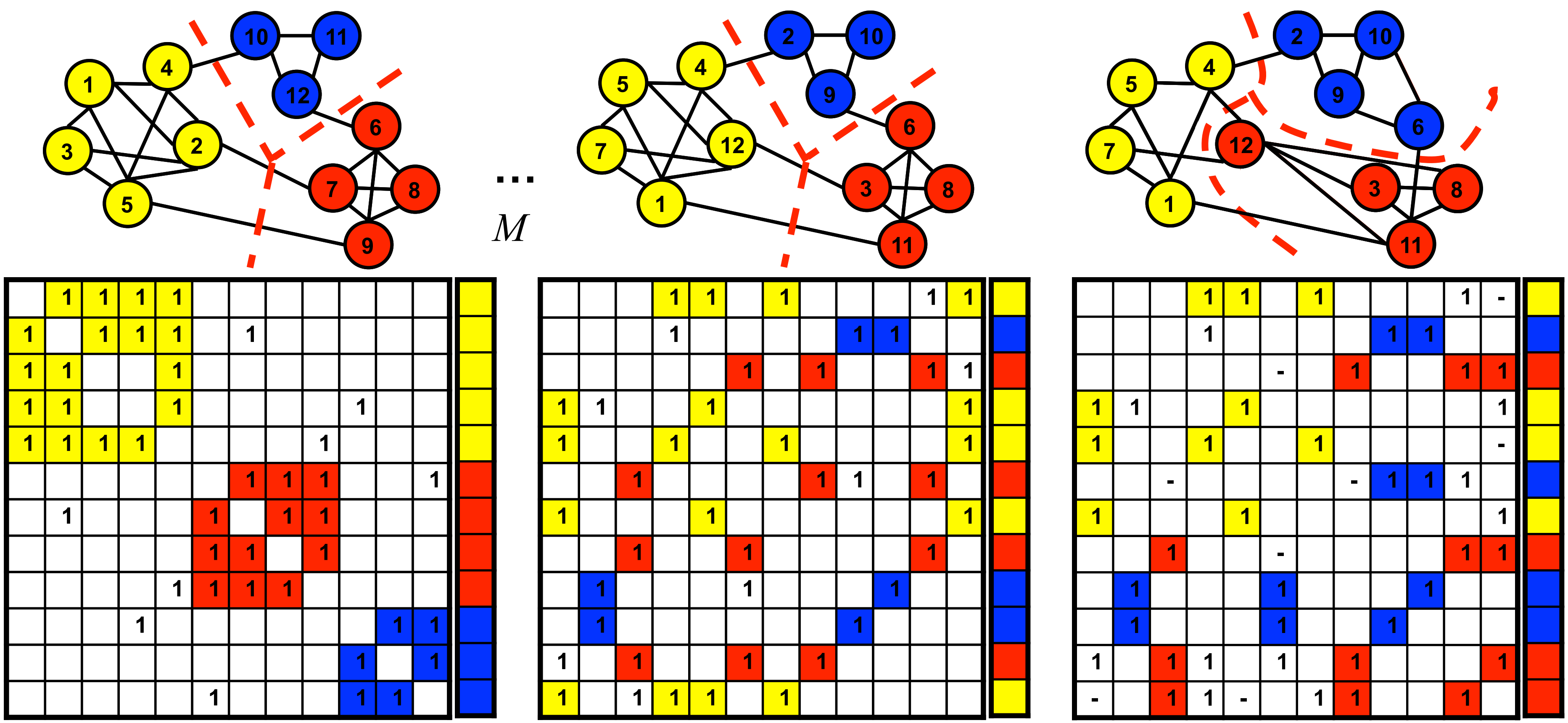


$$\mathbb{T}(\tilde{c}) = \{\tau : \forall \beta, c, w_\beta(c, \mathbf{X}) = w_\beta(\tau \circ c, \tau \circ \mathbf{X}) \ \wedge \ D(w_\beta(., \mathbf{X}), w_\beta(., \tau \circ \mathbf{X})) > \rho\}$$

Code problem generation for graph cut

graph cut *code* problems

graph cut *test* problem



Communication process and decoding

- Sender sends transformation τ_s
- Receiver accepts instance $\tilde{\mathbf{X}} := \tau_s \circ \mathbf{X}''$ with $\mathbf{X}', \mathbf{X}'' \sim P(\mathbf{X})$ and decodes the transformation by **maximizing expected posterior**

$$\hat{\tau} \in \arg\max_{\tau \in \mathcal{T}} \mathbb{E}_{\tilde{c}|\tau \circ \mathbf{X}'} \, p(\tilde{c}|\tau_s \circ \mathbf{X}'')$$

- **Error** event: $\hat{\tau} \neq \tau_s$

Generalization capacity from typicality

- **Theorem**: Asymptotic error free *identification* $\lim_{n\to\infty} P(\hat{\tau} \neq \tau_s | \tau_s) = 0$ of *code structures* is possible for

$$P\left(\hat{\tau} \neq \tau_s | \tau_s\right) \;\leq\; M\, \mathbb{E}_{\mathbf{X}',\mathbf{X}''} \Big(|\mathbb{T}| k^{\mathcal{A}}(\mathbf{X}', \mathbf{X}'') \Big)^{-1}$$

$$\overset{\text{typicality}}{\leq} \;\exp\Big(-(\mathcal{I} - \log M) \Big) \qquad \text{with}$$

$$\mathcal{I} \;=\; \mathbb{E}_{\mathbf{X}',\mathbf{X}''} \log\Big(|\mathbb{T}| k^{\mathcal{A}}(\mathbf{X}', \mathbf{X}'') \Big)$$

$$k^{\mathcal{A}}(\mathbf{X}', \mathbf{X}'') \;=\; \sum_{c\in\mathcal{C}} p^{\mathcal{A}}(c|\mathbf{X}') p^{\mathcal{A}}(c|\mathbf{X}'') \in [0,1]$$

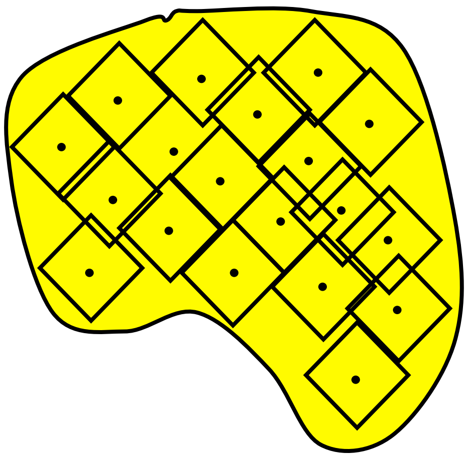
Behavior of the generalization capacity

- Let us assume that $\mathbf{X}', \mathbf{X}''$ are very similar.

$$\mathbf{X}' \approx \mathbf{X}'' \approx \mathbf{X}$$

$$k^{\mathcal{A}}(\mathbf{X}, \mathbf{X}) = \sum_{c \in \mathcal{C}} p^{\mathcal{A}}(c|\mathbf{X})^2 = \frac{|A_{t^*}(\mathbf{X}) \cap A_{t^*}(\mathbf{X})|}{|A_{t^*}(\mathbf{X})|^2}$$

$$\mathcal{I} = \mathbb{E}_{\mathbf{X}} \log\Big(\frac{|\mathbb{T}|}{|A_{t^*}(\mathbf{X})|}\Big)$$



- 2nd order terms yield maximum of GC $\mathcal{I}$ for parameter selection

Learning an algorithm: open challenge!

- **Statistical behavior of an algorithm** is described by its posterior $p^{\mathcal{A}}(c|\mathbf{X}')$
- **Adapt posterior** $p^{\mathcal{A}}(c|\mathbf{X}')$ s.t. generalization capacity is maximized

$$p^* \in \arg \max_{\substack{p^{\mathcal{A}}:\mathcal{X}\times\mathcal{C}\to[0,1] \\ \sum_c p^{\mathcal{A}}(c|\mathbf{X})=1}} \mathbb{E}_{\mathbf{X}',\mathbf{X}''} \log\Big(|\mathbb{T}|\, k^{\mathcal{A}}(\mathbf{X}',\mathbf{X}'')\Big)$$

- **Problem**: We cannot evaluate $\mathbb{E}_{\mathbf{X}',\mathbf{X}''} \log \ldots$ since $P(\mathbf{X}',\mathbf{X}'')$ is unknown!

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Example: Robust Spanning Trees

- **Given** are graphs with stochastic edge weights.
- **Question**: How robust are MST algorithms in this stochastic setting?
- Measure **robustness of algorithms** like Prim's, Kruskal's algorithm or the Reverse-Delete algorithm.
- Determine a **stable set of approximate spanning trees** by early stopping of an MST algorithm.

Learning to span a graph

Alexey Gronskiy

Consider **Minimum Spanning Tree** algorithms

- **Prim**’s “Growing tree” strategy: add minimal edge to tree.
- **Kruskal**’s “Joining trees” strategy: add minimal edge connecting two trees in a forest.
- **Reverse-Delete**: “Reducing graph” strategy: delete maximal edge without destroying connectivity.

MST Algorithm as a sequence of approximate spanning tree sets

- Let $\mathbf{X}$ be a graph and $A_t(\mathbf{X})$ the set of spanning trees at iteration t

$$\begin{aligned} \mathcal{A}(\mathbf{X}) &= \langle A_0(\mathbf{X}), \ldots, A_T(\mathbf{X}) \rangle, \\ A_t(\mathbf{X}) &\subseteq \mathcal{C}, \quad 0 \leq t \leq T, \\ A_0(\mathbf{X}) &= \mathcal{C}, \quad A_T(\mathbf{X}) = \{c^\perp\}. \end{aligned}$$

- Monotonically contractive algorithms

$$\mathcal{A}(\mathbf{X}) = \langle A_0(\mathbf{X}) \supseteq A_1(\mathbf{X}) \supseteq \ldots \supseteq A_T(\mathbf{X}) \rangle$$

Cardinality of AST sets

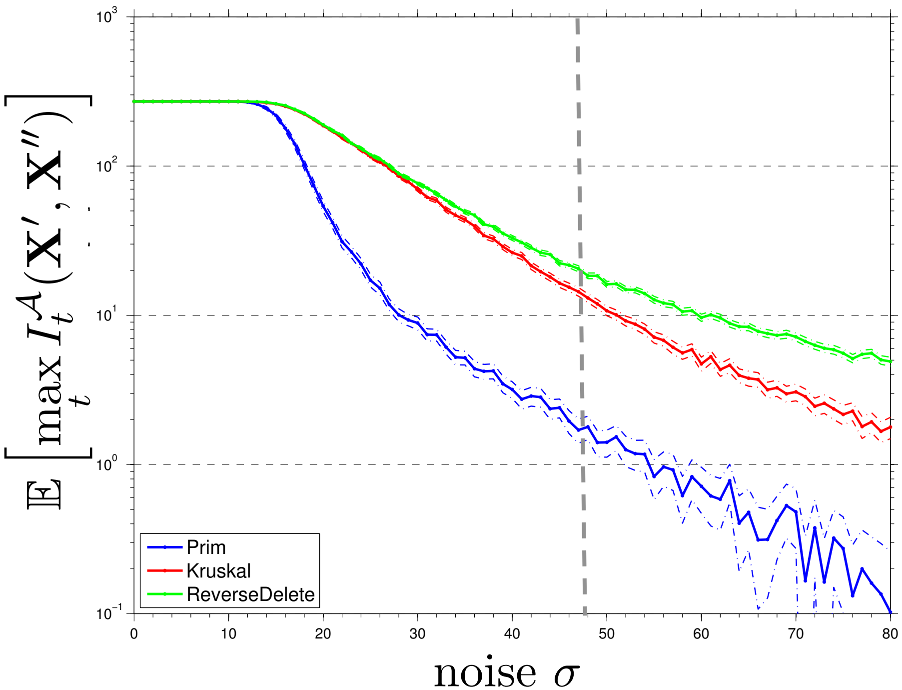
- **Matrix tree theorem**: the number of spanning trees is equal to (any) cofactor of the matrix

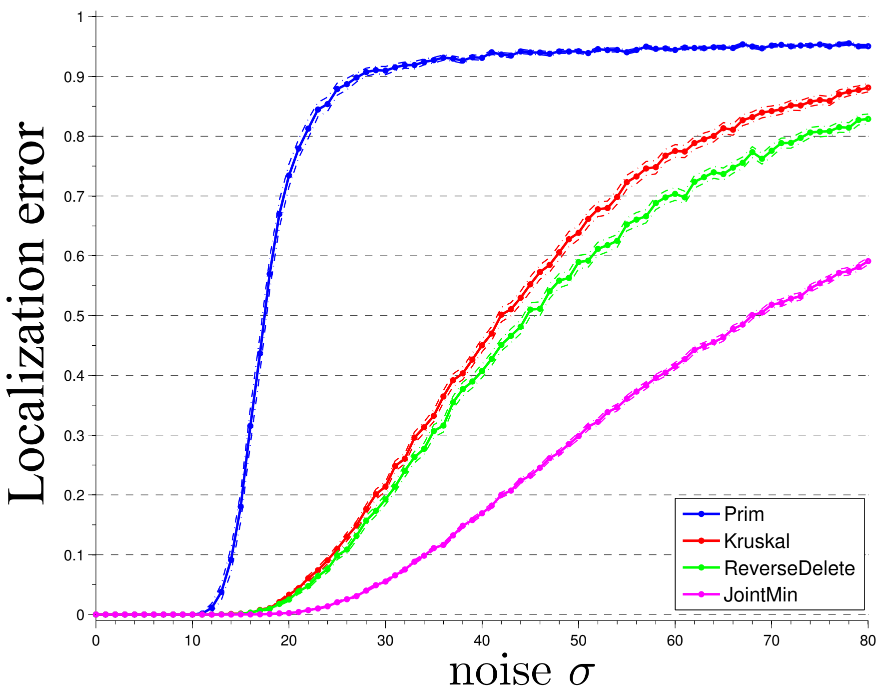
$$L = M_{\text{deg}}^{X} - M_{\text{adj}}^{X}$$

- Calculate the cofactor of L after t steps for the effective $X(t)$ where selected edges are contracted (Prim, Kruskal) or removed (Reverse-Delete).

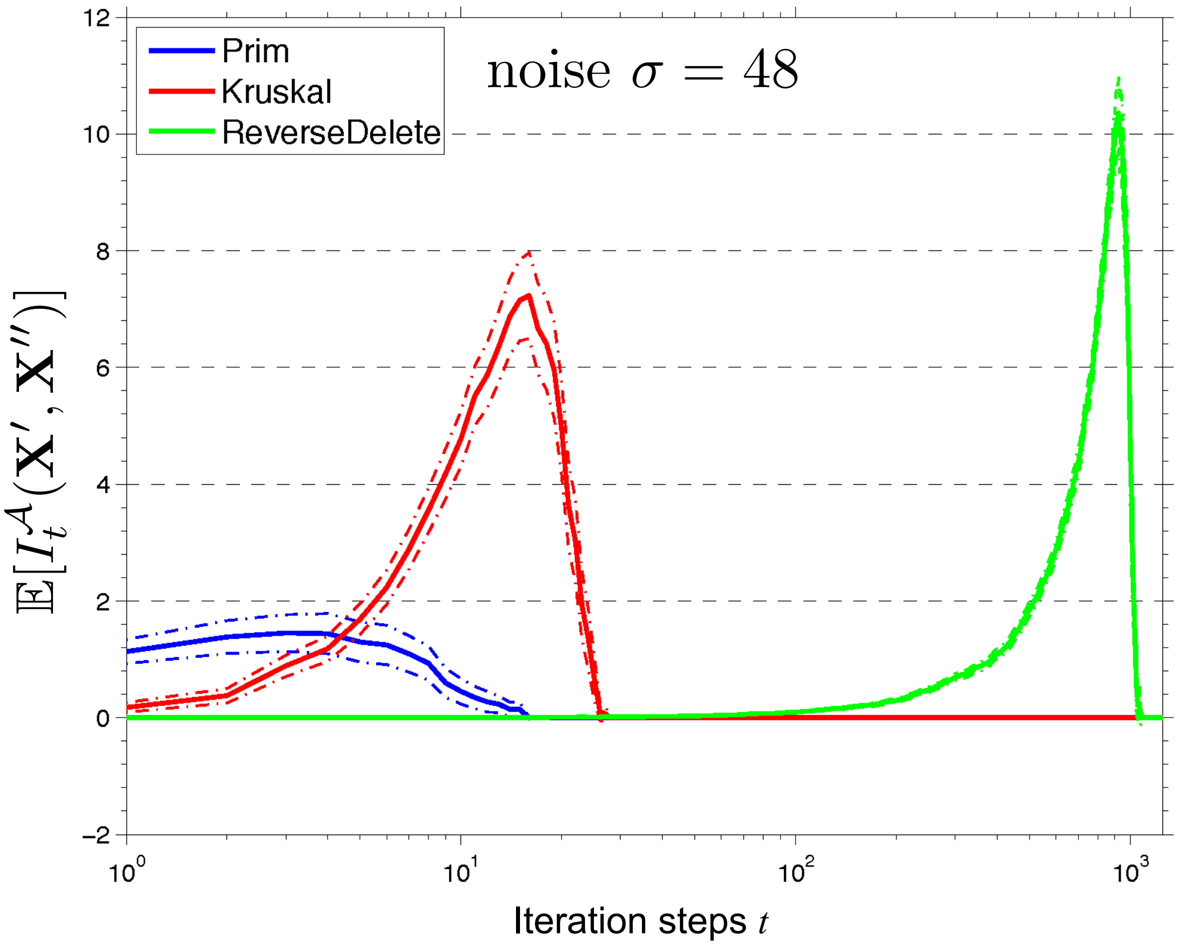
Algorithmic informativeness

- Hierarchical graph generation:
  - ground truth graph: 50 vertices, i.i.d. normal weights $\mathcal{N}(100, 100)$
  - Additive Gaussian noise $\mathcal{N}(0, \sigma^2) \;\Rightarrow\; \mathbf{X}', \mathbf{X}''$



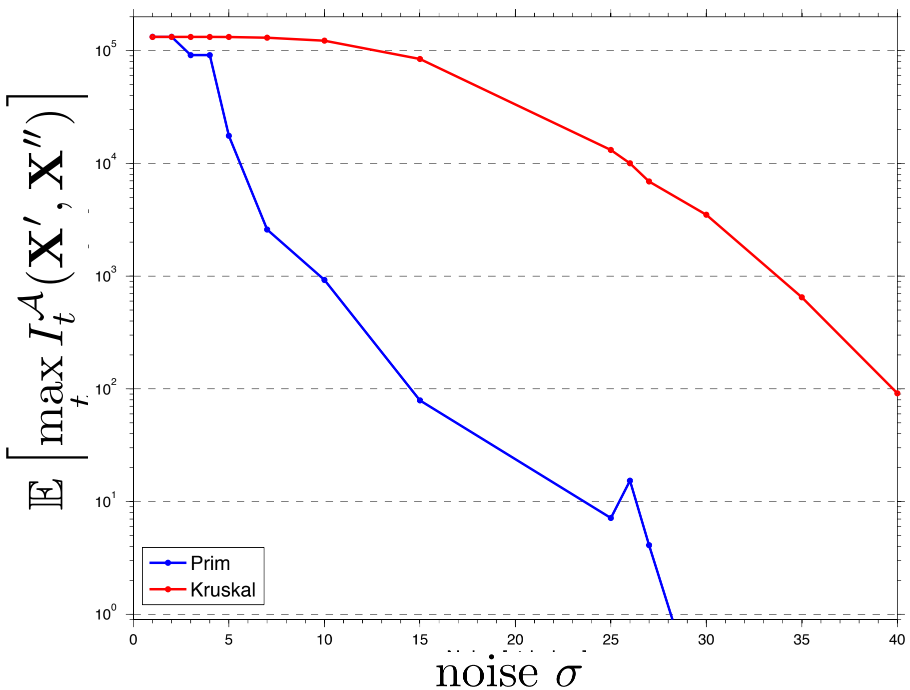


Dynamics of algorithmic informativeness



Informativeness of ASTs with 10^4 vertices

- Hierarchical graph generation:
  - ground truth graph: 10^4 vertices, i.i.d. normal weights $\mathcal{N}(100, 100)$
  - Additive Gaussian noise $\mathcal{N}(0, \sigma^2)$



Conclusion

- **Quantization**: Noise quantizes mathematical structures (hypothesis classes) **=>** symbols
- **Coding** with these symbols defines a **generalization capacity** for **algorithms**

$\Rightarrow$ **Quantization** of hypothesis class measures **structure specific information** in data.

- How to relate **statistical complexity** to algorithmic or **computational complexity** ?