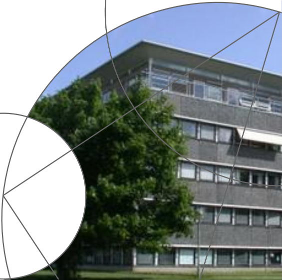
Faculty of Science

Greedy Learning of Causal Structures in Additive Noise Models

Master thesis defense

Phillip Bredahl Mogensen
Department of Mathematics

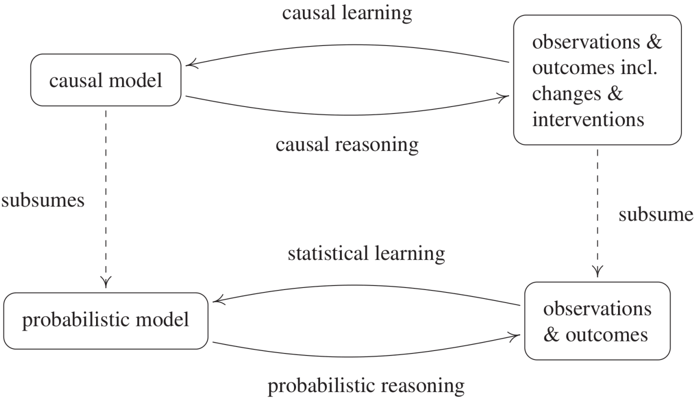


Agenda

1. Causal discovery and Additive Noise Models
2. Entropy scores and the Greedy entropy-search
3. A few simulations and real data
4. Conclusion

Causal discovery and Additive Noise Models

Aim of the thesis



Source: Peters et al. 2017, Page 6.

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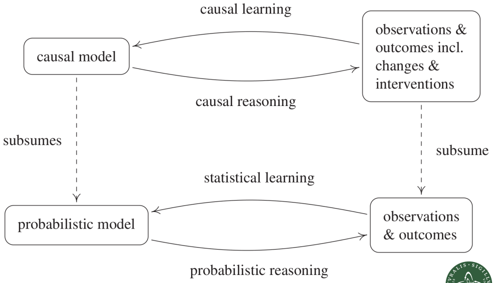

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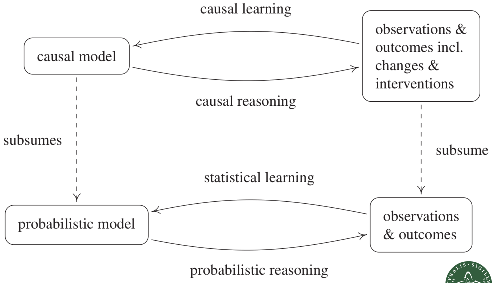

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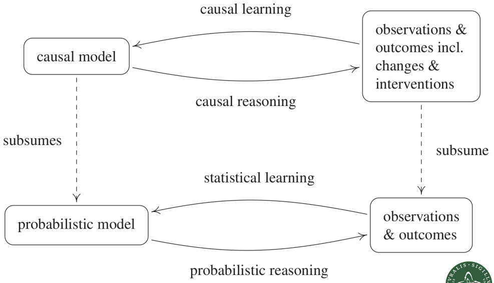

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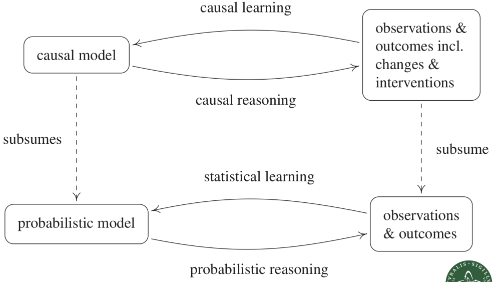

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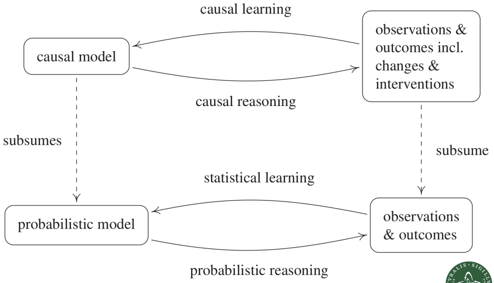

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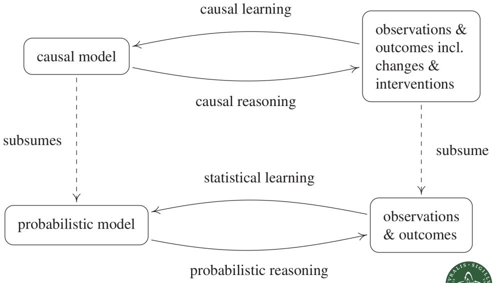

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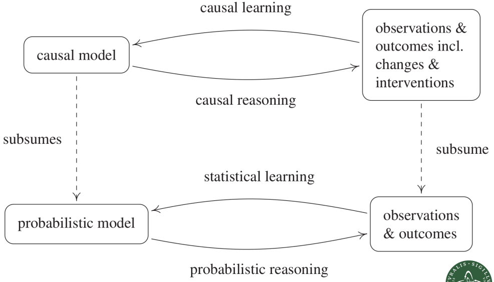
- Additive Noise Models.
- A score-based Greedy search.



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- To get identifiability, we lean on existing results

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(A3) The densities of the noise variables have only discretely many solutions to the differential equation $(\log f)'' = 0$.

(A4) The noise variables have full support and their densities are in C^3 and strictly positive.

(A5,6) All noise variables and all $\mathcal{F}$-transformations of them have second moment.

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Entropy scores and the Greedy entropy-search

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Q: Why this score function?

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- **Implication:** To find $\mathcal{G}^0$, just maximize ℓ.
- We just check every possible graph!

The problem

How many graphs do we need to check if we have p variables?

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Too many! Computationally an impossible task.
Instead, we do a Greedy search.

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Getting to optimality – prerequisites

A few technicalities

- Introduce the Gaussian score:

$$\ell^{g}(\mathcal{G}) := -\sum_{\nu \in V(\mathcal{G})} \log \mathbb{V}\left(\text{residuals of } X_{\nu}\right)$$

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All parents are mutually independent

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All cycles have at least three colliders

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- **A:** Yes!

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- **Q:** Can we be sure it gives a global optimum?
- **A:** Yes! But it requires a bit of work.

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Includes (A1)–(A6). The rest we find during the proof

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- To get there, we rely on three results.

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Prerequisites

Proposition 5

Let $\mathscr{C}$ be an ANM with graph $\mathcal{G}^0$ and let $\mathcal{G}$ be a subgraph. If $\alpha \perp_d \beta \mid \mathbf{PA}_{\mathcal{G}}(\beta)$, then

$$\Delta\ell^g(\mathcal{G}, \alpha \to \beta) = 0.$$

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Proposition 6

Same set-up as above. If $\alpha \to \beta$ is in $\mathcal{G}^0$ but not in $\mathcal{G}$, then

$$\Delta\ell^g(\mathcal{G}, \alpha \to \beta) > 0.$$

Proving optimality – part one

Prerequisites continued

Lemma 7

Let $(X, Y) \sim \mathbb{P}_{(X,Y)}$ *and* $N \sim \mathbb{P}_N$ *with* $N \perp\!\!\!\perp Y$*.*

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Let $(X, Y) \sim \mathbb{P}_{(X,Y)}$ *and* $N \sim \mathbb{P}_N$ *with* $N \perp\!\!\!\perp Y$. *Assume that* $x \mapsto \mathbb{E}_N f(g(x) + N)$ *is in* $\mathcal{F}$ *whenever* $f, g \in \mathcal{F}$.

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$$\min_{f \in \mathcal{F}} \mathbb{E}_{(X,Y)} (Y - f(X))^2 < \min_{f \in \mathcal{F}} \mathbb{E}_{(X,Y,N)} (Y - f(g(X) + N))^2$$

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Intuition:

MSE of regressing Y onto X $<$
MSE of regressing Y onto noisy version of X.

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- Divide into three cases.
  1. α and β are not *d*-connected in $\mathcal{G}^0$.
  2. α and β are *d*-connected in $\mathcal{G}^0$ through $\mathbf{PA}_{\mathcal{G}^0}(\alpha)$.

Proving optimality – part one

- We are now ready to prove part one.
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- Case 3 turns out to follow from case 2.

Proving optimality – part one

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- Observe: There is only one *d*-connection, ϵ, between α and β.

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    - Otherwise, there would be a cycle with < 3 colliders.
- We let π be the parent of α on ϵ and ρ be the neighbor of β along ϵ.

Proving optimality – part one

Case 2 continued:

Suppose first that ρ is a parent of β.

Proving optimality – part one

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\begin{tikzcd}
\Omega_\beta \arrow[d] & & & \Omega_\alpha \setminus \{\pi\} \arrow[d] \\
\beta & \rho \arrow[l, dashed] \arrow[r, leftrightsquigarrow, "d"] & \pi \arrow[r, dashed] & \alpha \\
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    - Boils down to exploiting the independence structure of $\mathscr{C}$. But we won't show this.

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- We then move on to part 2.

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$$\begin{array}{ccc} \mathbf{PA}_{\mathcal{G}^s}(\beta) & \qquad & \mathbf{PA}_{\mathcal{G}^s}(\alpha) \\ \downarrow & & \downarrow \\ \beta & & \alpha \end{array}$$

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  - We then apply Theorem 3 to reach a contradiction.

$$\begin{tikzcd} \mathbf{PA}_{\mathcal{G}^s}(\beta) \arrow[d] & \mathbf{PA}_{\mathcal{G}^s}(\alpha) \arrow[d] \\ \beta \arrow[r] & \alpha \end{tikzcd}$$

Theorem 3

If $\mathcal{G}^0$ is the true graph of an ANM that satisfies (A1)–(A6), then

$$\mathcal{G}^0 = \arg\max_{\mathcal{G}} \ell(\mathcal{G}).$$

Proving optimality – part two

Difficulties in proving part two

- To apply Theorem 3, we need $\tilde{\mathcal{G}}$ to be the graph of an identifiable ANM, $\tilde{\mathscr{C}}$.

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- Notice that the $\tilde{N}$ variables are mutually independent.

Proving optimality – part two

(A1,2) $\mathcal{F}$ consists of non-linear C^3 functions + some regularity conditions.

(A3) The densities of the noise variables have only discretely many solutions to the differential equation $(\log f)'' = 0$.

(A4) The noise variables have full support and their densities are in C^3 and strictly positive.

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- $(\log f)'' = 0 \Leftrightarrow f(x) = exp(c_1 \cdot x + c_2)$.
- We call these functions **log-linear**.

Proving optimality – part two

Solving the convolution problem

Lemma 8

Let f be a real analytic function.

Proving optimality – part two

Solving the convolution problem

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Let f be a real analytic function.

C^∞ and has a convergent power series representation in a neighborhood of every point. Symbol: C^ω.

Proving optimality – part two

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Let f be a real analytic function. If f is log-linear on $[a, b]$, then f is log-linear on all of $\mathbb{R}$.

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Let $f \in C^\omega \cap \mathcal{L}^\infty$ and $g \in \mathcal{L}^1$.

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Theorem 9

Let $f \in C^\omega \cap \mathcal{L}^\infty$ and $g \in \mathcal{L}^1$. Then $f * g \in C^\omega$.

Proving optimality – part two

Solving the convolution problem continued

Corollary 10

Let $f \in C_{+}^{\omega}$ and $g \in \mathcal{L}^{\infty}$ be densities.

Proving optimality – part two

Solving the convolution problem continued

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Let $f \in C_+^\omega$ and $g \in \mathcal{L}^\infty$ be densities. The convolution $f * g$ is not log-linear on any interval.

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Proof.

1. Observe that $f * g$ is integrable and real analytic.

□

Proving optimality – part two

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Proof.

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3. $h(x)$ is not real analytic $\Rightarrow f * g$ is not log-linear on all of $\mathbb{R}$.
4. $\Rightarrow f * g$ is not log-linear on any interval.

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Proving optimality – part two

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Let $f \in C_+^\omega$ and $g \in \mathcal{L}^\infty$ be densities. The convolution $f * g$ is not log-linear on any interval.

- **Implication:** All N's have real analytic densities $\Rightarrow$ all $\tilde{N}$'s satisfy (A3).

Proving optimality – part two

Solving the convolution problem continued

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Let $f \in C^{\omega}_{+}$ and $g \in \mathcal{L}^{\infty}$ be densities. The convolution $f * g$ is not log-linear on any interval.

- **Implication:** All N's have real analytic densities $\Rightarrow$ all $\tilde{N}$'s satisfy (A3).
- Includes Gaussian variables, among others.

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- $\tilde{\mathscr{C}}$ is now identifiable!

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- By Theorem 3

$$\ell(\tilde{\mathcal{G}}) > \ell(\tilde{\mathcal{G}}_{\alpha\to\beta})$$

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- Write out and rearrange...

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$$\ell(\tilde{\mathcal{G}}) > \ell(\tilde{\mathcal{G}}_{\alpha \to \beta})$$

- Write out and rearrange...
- We get

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- **Remark:** Proof can be made to work with linear assignments.

A few simulations and real data

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- Non-parametric regression with `gam` from `mgcv` package.

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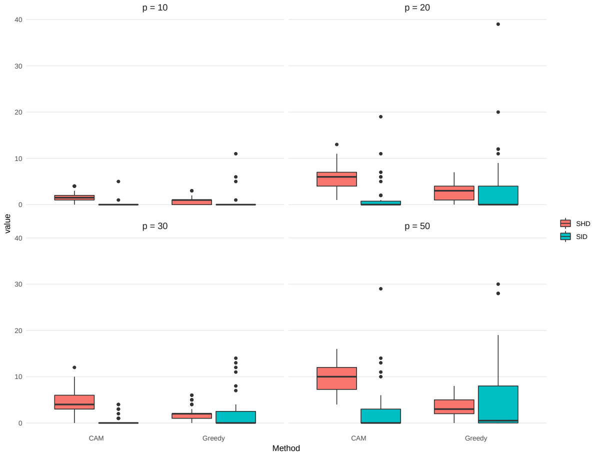
Non-linear, Gaussian case

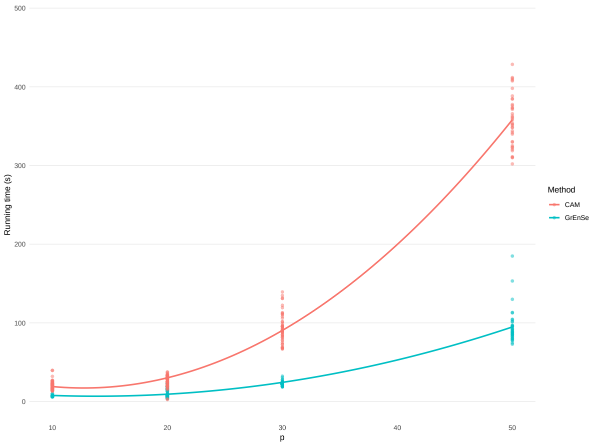
Comparison to CAM



50 repetitions, $N = 300$. p is number of nodes.

Non-linear, Gaussian case

Comparison to CAM – computation time



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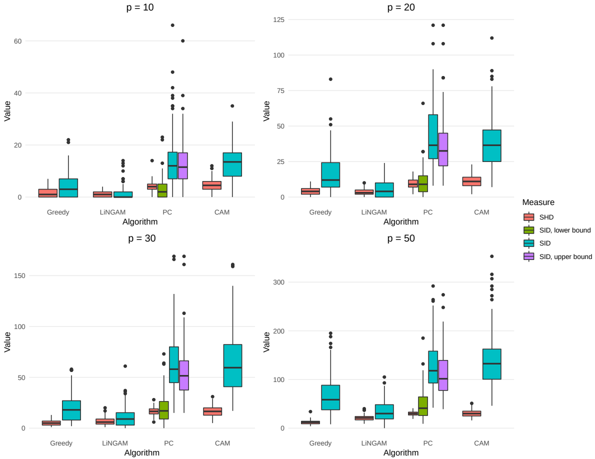
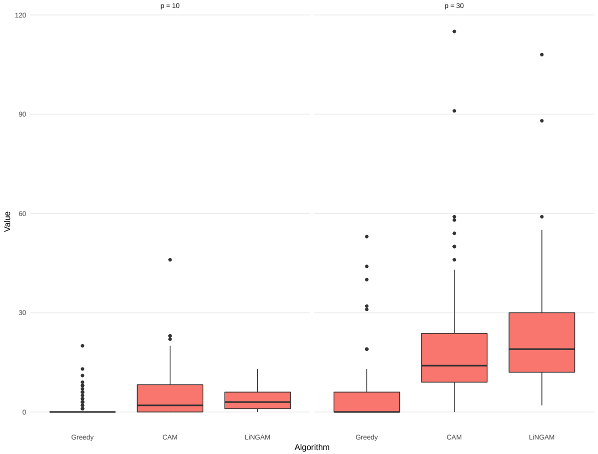
Comparison to other other methods



100 repetitions, $N = 1000$. p is number of nodes. Noise is Hyperbolic Secant

Non-Gaussian, no assumption on linearity

Comparison to other other methods – only SID



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- Simulations were small-scale.
- We did not attempt to optimize runtimes with CAM – could possibly be sped up.

Future work

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- Relax assumptions of main proof.

Thanks for listening ☺

Proof of Lemma 7

Proof.

Choose any $f, g \in \mathcal{F}$. By Jensen's inequality

$$(Y - \mathbb{E}_N f(g(X) + N))^2 < \mathbb{E}_N (Y - f(g(X) + N))^2.$$

Take $\mathbb{E}_{(X,Y)}$ on both sides and use Tonelli:

$$\mathbb{E}_{(X,Y)}(Y - \mathbb{E}_N f(g(X) + N))^2 < \mathbb{E}_{(X,Y,N)}(Y - f(g(X) + N))^2.$$

By assumption, this implies:

$$\min_{f \in \mathcal{F}} \mathbb{E}_{(X,Y)}(Y - f(X))^2 < \min_{f \in \mathcal{F}} \mathbb{E}_{(X,Y,N)}(Y - f(g(X) + N))^2.$$

$\square$

Proof of Lemma 8

Proof.

Assume for contradiction that f does not solve $(\log f)'' = 0$ on $\mathbb{R} \backslash [a, b]$. By assumption

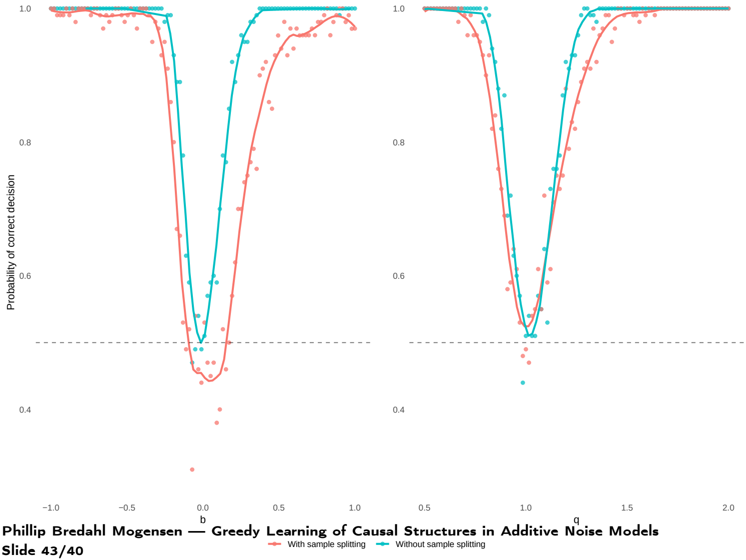
$$\forall n \in \mathbb{N}_0 : \quad f^{(n)}(a) = \exp(c_2) \cdot c_1^n \cdot \exp(c_1 \cdot a) =: \tilde{k} \cdot c_1^n.$$

Taylor-expand f around a:

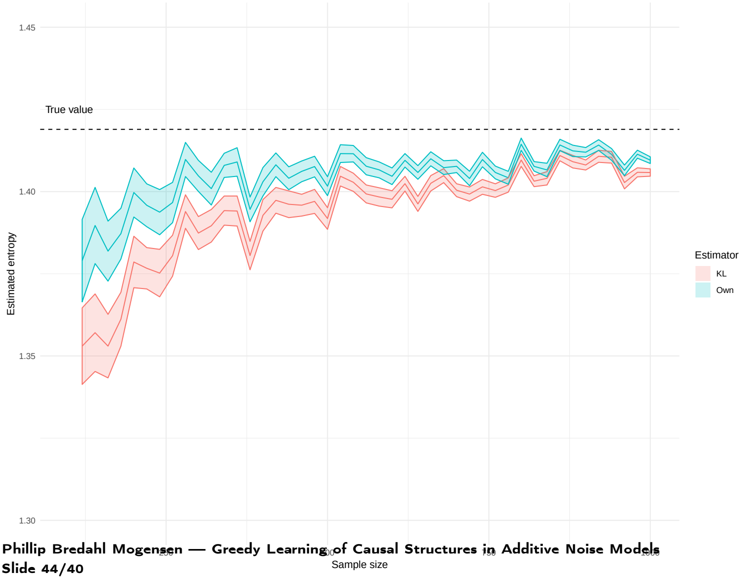
$$f(x) = \cdots = \tilde{k} \sum_{i=0}^{\infty} \frac{c_1^i}{i!}(x-a)^i = \tilde{k} \exp(c_1 \cdot (x-a)).$$

This holds in an open neighborhood of a, which gives us a contradiction. □

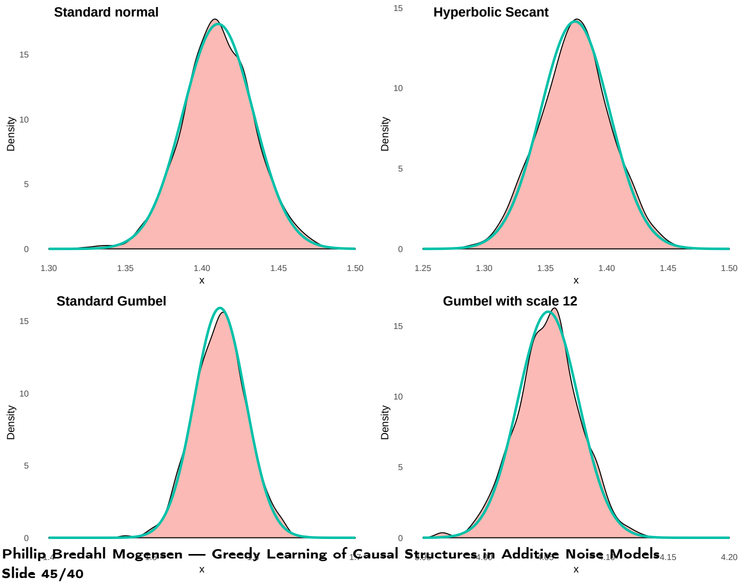
Bivariate case



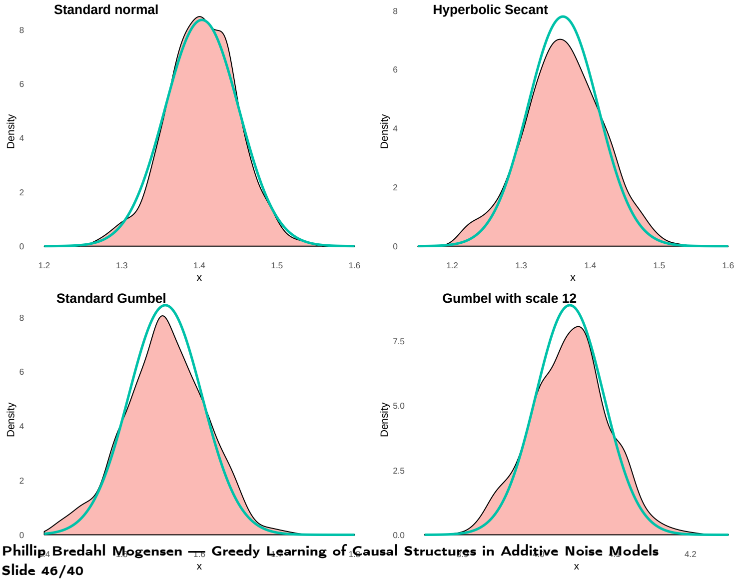
KL vs. logspline estimation



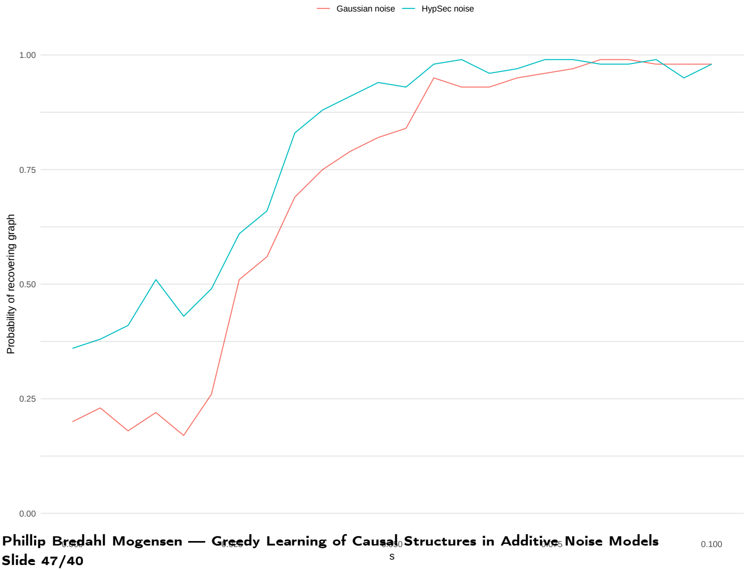
Asymptotics of entropy estimator



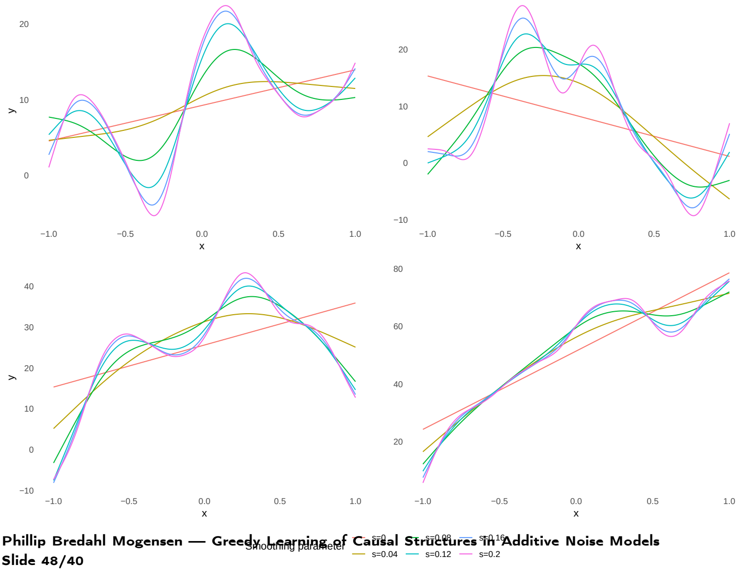
Asymptotics of entropy estimator, $n = 250$



Linear assignments



Examples of random functions



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Jonas Martin Peters, Dominik Janzing, and Bernhard Schölkopf. *Elements of causal inference, foundations and learning algorithms*. Adaptive computation and machine learning series. MIT Press, Cambridge, MA, 2017. ISBN 9780262037310.