Totally Concave Regression

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Joint work with Aditya Guntuboyina

We propose a new multivariate generalization of univariate concave regression.

Our new method is based on total concavity.

Total concavity is a multivariate extension of univariate concavity, defined via max-order mixed (partial) derivative constraints.

Univariate Concave Regression

Data: $(x^{(1)}, y_1), \ldots, (x^{(n)}, y_n)$ where $x^{(i)} \in [0,1]$ and $y_i \in \mathbb{R}$

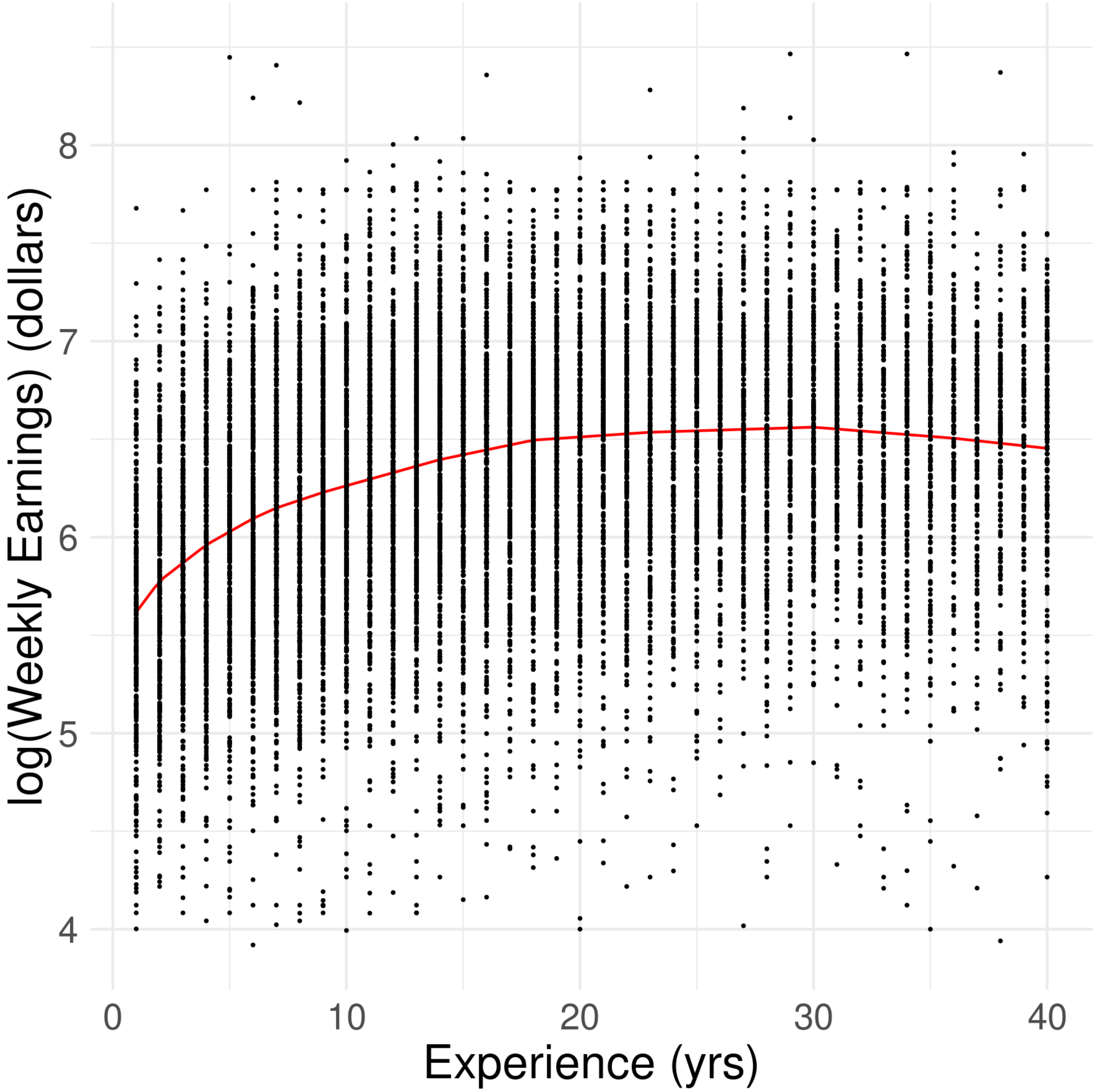
Suppose y has diminishing returns with respect to x.

In other words, the rate of change in y decreases as x increases.

$(= dy/dx)$

$$\hat{f}_{\text{concave}} \in \underset{f:\text{concave}}{\operatorname{argmin}} \sum_{i=1}^{n} \left(y_i - f(x^{(i)})\right)^2$$

Example



log(Weekly Earnings) (dollars)
8
7
6
5
4
0
10
20
30
40
Experience (yrs)

Multivariate Concave Regression

What are multivariate versions of $\hat{f}_{\text{concave}}$?

For simplicity, we mainly focus on the bivariate case $d = 2$.

Data: $(x^{(1)}, y_1), \ldots, (x^{(n)}, y_n)$ where $x^{(i)} \in [0,1]^2$ and $y_i \in \mathbb{R}$

Example: $y = \log(\text{Earnings})$, $x_1 = \text{Education}$, and $x_2 = \text{Experience}$.

Existing Notions of Multivariate Concavity

- General Concavity

- Axial (= Coordinate-wise) Concavity

- Additive Concavity

Total concavity is different from them!

General Concavity

f is (generally) concave if and only if

$$f((1-\alpha)x + \alpha y) \geq (1-\alpha)f(x) + \alpha f(y)$$

for all $\alpha \in [0,1]$ and $x, y \in [0,1]^2$.

Studied in, for example,

[Balázs 2016], [Kuosmanen 2008], [Lim & Glynn 2012],

[Seijo & Sen 2011], [Kur et al 2024], ...

Weakness:

It requires concavity on every line $\gamma_0 + \gamma_1 x_1 + \gamma_2 x_2 = 0$.

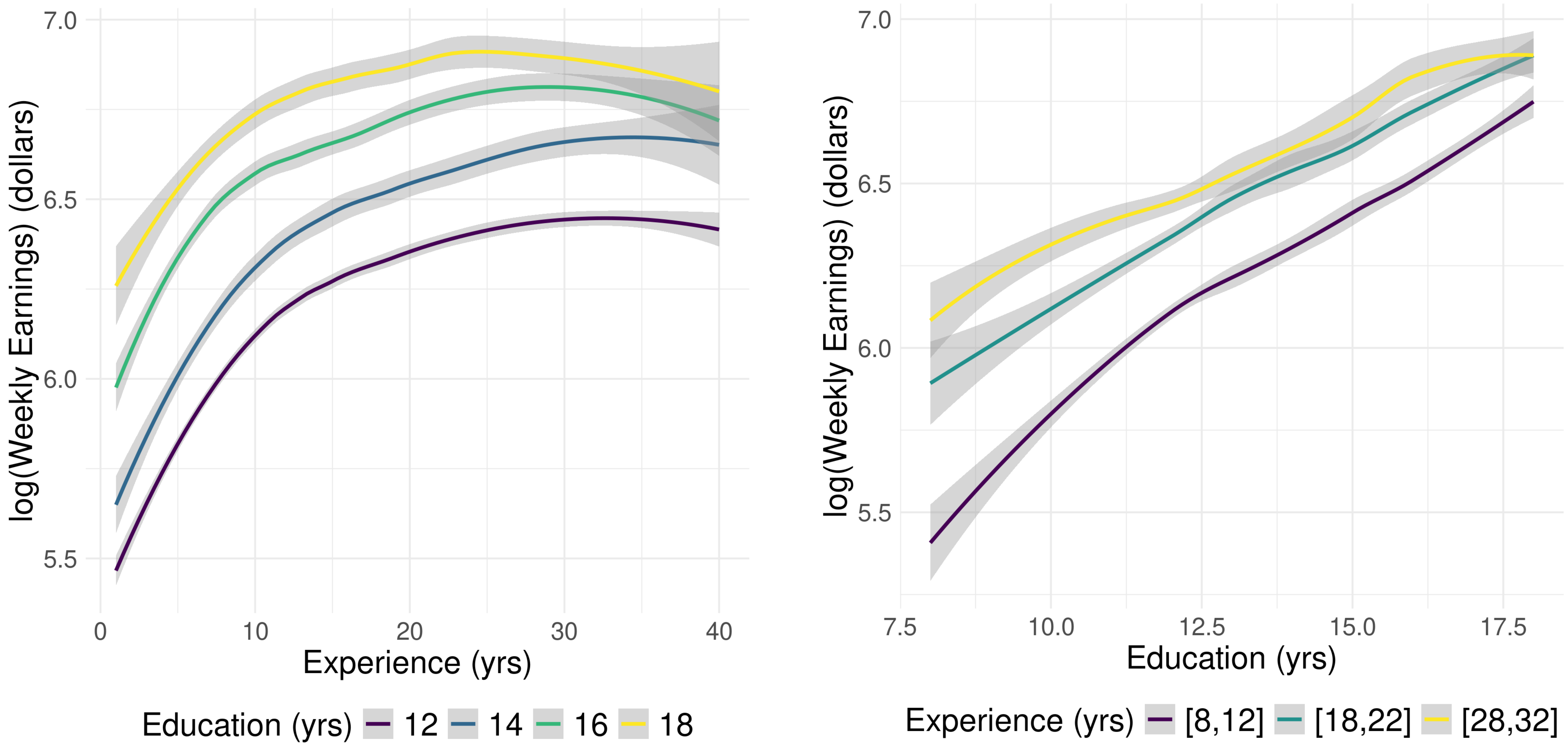
Axial Concavity

f is axially (coordinate-wise) concave if and only if

$f(\cdot, x_2)$ and $f(x_1, \cdot)$ are concave for each $x_1, x_2 \in [0,1]$.

It is often justifiable from domain knowledge or data.

Example



7.0
6.5
6.0
5.5
log(Weekly Earnings) (dollars)
0
10
20
30
40
Experience (yrs)
Education (yrs) 12 14 16 18
7.0
6.5
6.0
5.5
log(Weekly Earnings) (dollars)
7.5
10.0
12.5
15.0
17.5
Education (yrs)
Experience (yrs) [8,12] [18,22] [28,32]

Axial Concavity

Studied in, for example, [Iwanaga et al 2016]

Weakness:

Axial concavity is a weak assumption.

It may require more data to avoid overfitting than others

Additive Concavity

f is additive concave if and only if

$f(x_1, x_2) = f_1(x_1) + f_2(x_2)$ for some univariate concave functions f_1 and f_2.

Studied, for example, in

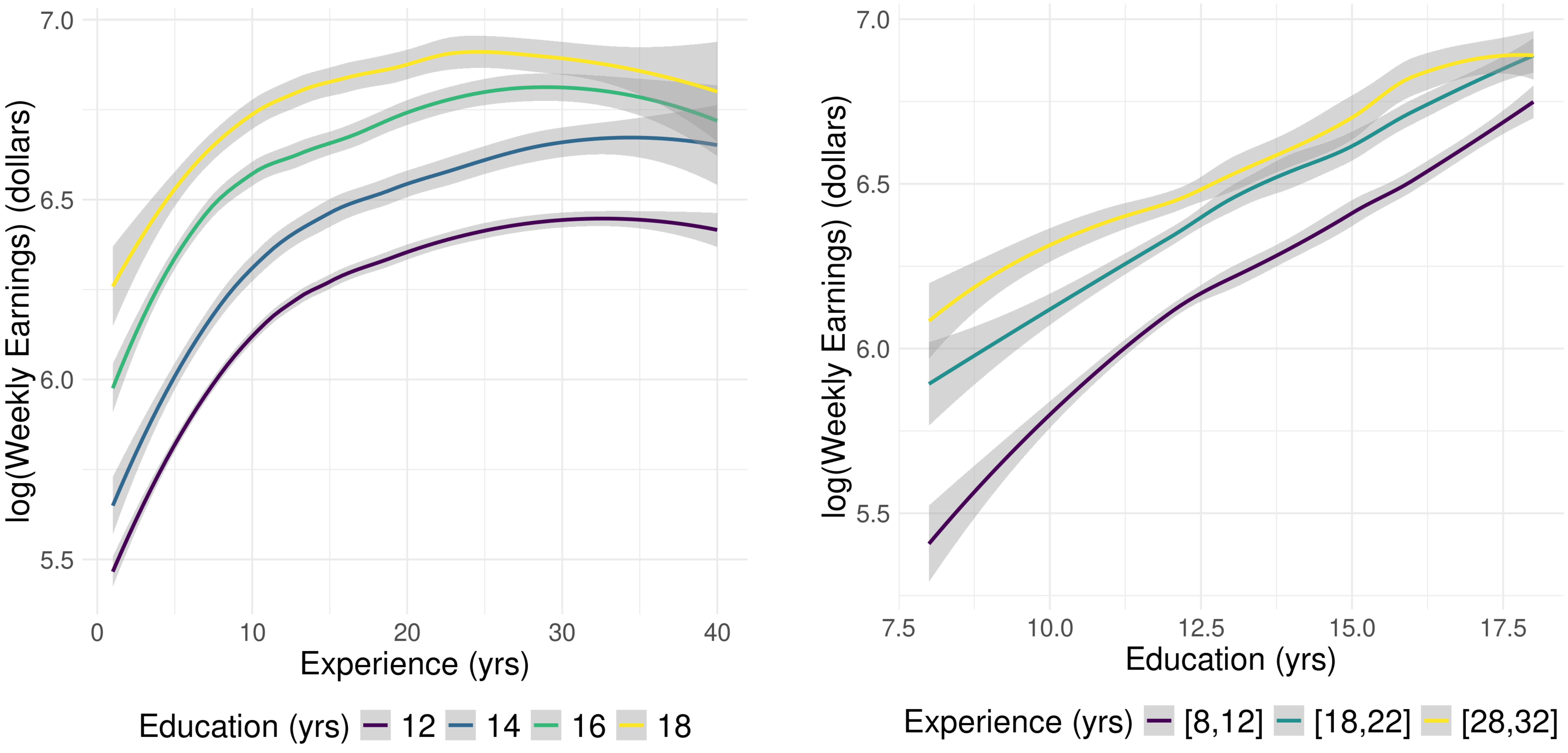
[Chen & Samworth 2016], [Meyer 2013], [Meyer 2018], [Pya & Wood 2015], ...

Weakness:

No interaction effects

Can be restrictive sometimes.

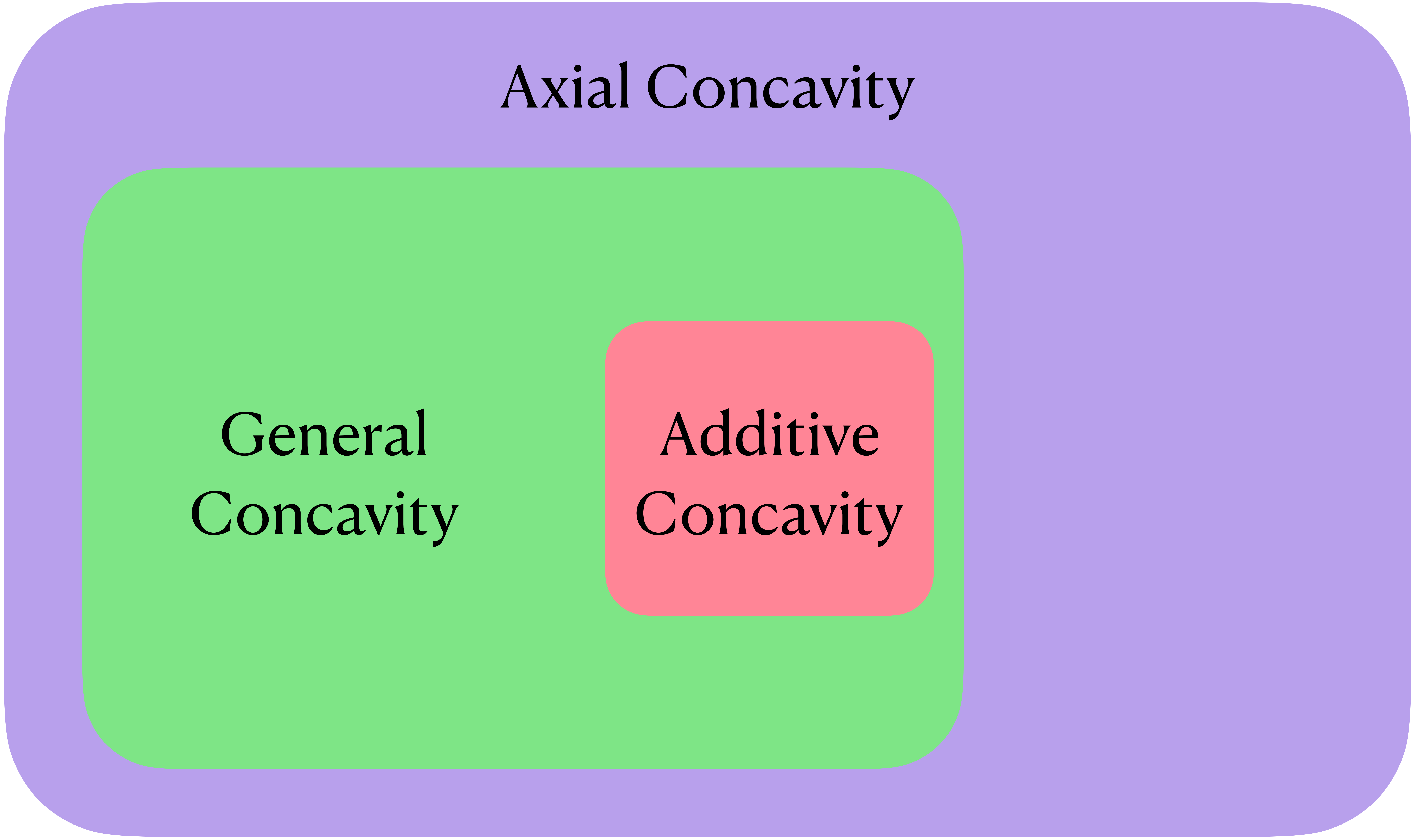
Example Again



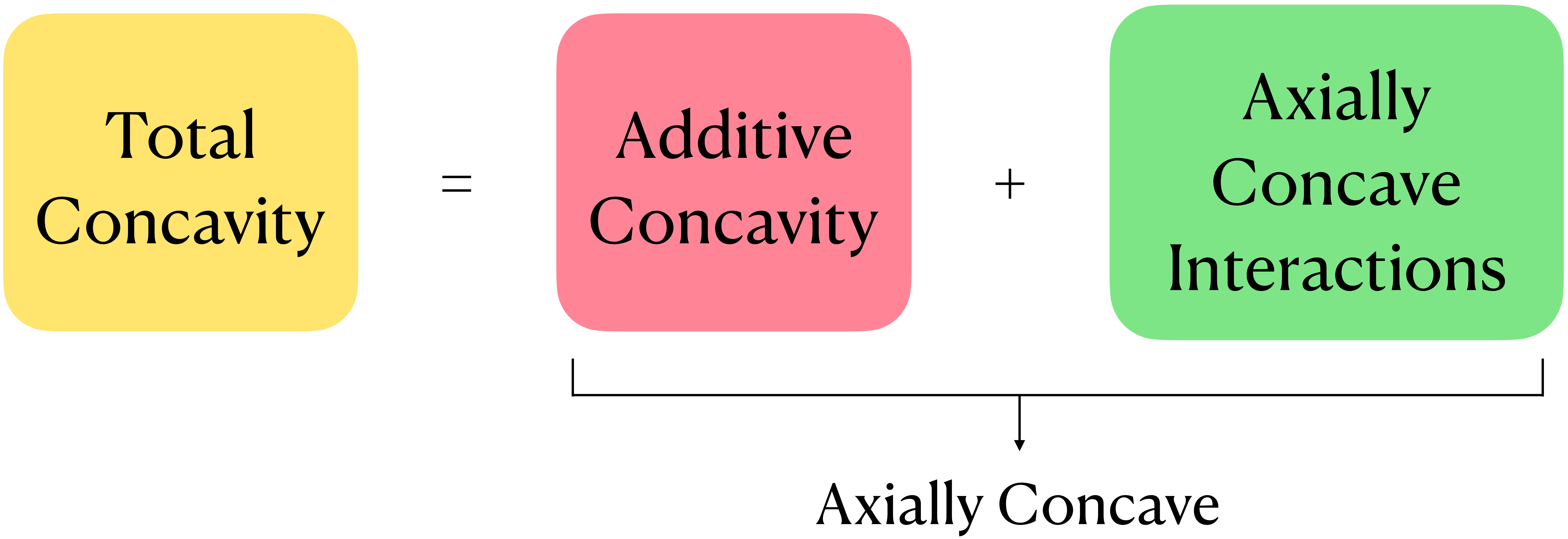
Characterization via Mixed (Partial) Derivatives

For smooth functions,

- Univariate Concavity: $f'' \leq 0$, i.e., $\dfrac{\partial^2 f}{\partial x_1^2} \leq 0$.
- General Concavity: $\dfrac{\partial^2 f}{\partial x_1^2} \leq 0$, $\dfrac{\partial^2 f}{\partial x_2^2} \leq 0$, and $\left(\dfrac{\partial^2 f}{\partial x_1 x_2}\right)^2 \leq \dfrac{\partial^2 f}{\partial x_1^2} \cdot \dfrac{\partial^2 f}{\partial x_2^2}$.
- Axial Concavity: $\dfrac{\partial^2 f}{\partial x_1^2} \leq 0$ and $\dfrac{\partial^2 f}{\partial x_2^2} \leq 0$.
- Additive Concavity: $\dfrac{\partial^2 f}{\partial x_1^2} \leq 0$, $\dfrac{\partial^2 f}{\partial x_2^2} \leq 0$, and $\dfrac{\partial^2 f}{\partial x_1 x_2} = 0$.


Axial Concavity
General Concavity
Additive Concavity

Total Concavity



First introduced by Popoviciu in 1934 and recently described in [Gal 2010].

Representation Theorem for Univariate Concave Functions

Suppose $f : [0,1] \to \mathbb{R}$ is a concave function with $f'(0+) < +\infty$ and $f'(1-) > -\infty$.

Then, there exists a unique (Borel) measure ν on $(0,1)$ and $a_0, a_1 \in \mathbb{R}$ such that for all $x \in [0,1]$,

$$f(x) = a_0 + a_1 x - \int_{(0,1)} (x - t)_+ \, d\nu(t),$$

where $(x - t)_+ = \max\{x - t,\ 0\}$.

Concave functions are (infinite) linear combinations of basis functions $x \mapsto (x - t)_+$ with non-positive weights.

Additive Concave Functions

Additive concave functions can be written as

$$f(x_1, x_2) = a_0 + a_1 x_1 + a_2 x_2 - \int_{(0,1)} (x_1 - t_1)_+ \, d\nu_1(t_1) - \int_{(0,1)} (x_2 - t_2)_+ \, d\nu_2(t_2)$$

for some measures ν_1 and ν_2 on $(0,1)$.

Total Concavity = Additive Concavity + Axially Concave Interactions

How can we add interaction terms to these additive concave functions?

Axially Concave Interactions

How do we introduce interaction terms to linear regression?

Example:

$$y = \beta_1 x_1 + \beta_2 x_2 \;\rightarrow\; y = \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

Interactions can be introduced via

$$x_1 x_2,\; x_1(x_2 - t_2)_+,\; (x_1 - t_1)_+ x_2,\; \text{and}\; (x_1 - t_1)_+(x_2 - t_2)_+$$

Total Concavity = Additive Concavity + **Axially Concave** Interactions

When are they axially concave?

- $\beta x_1 x_2$: axially concave for all $\beta \in \mathbb{R}$.
- $\beta x_1 (x_2 - t_2)_+$, $\beta (x_1 - t_1)_+ x_2$, $\beta (x_1 - t_1)_+ (x_2 - t_2)_+$: axially concave iff $\beta \leq 0$.

Totally Concave Functions

$$f(x_1, x_2) = a_0 + a_1 x_1 + a_2 x_2 - \int (x_1 - t_1)_+ \, d\nu_1(t_1) - \int (x_2 - t_2)_+ \, d\nu_2(t_2)$$

$$+ a_{12} x_1 x_2 - x_1 \cdot \int (x_2 - t_2)_+ \, d\nu_{1=0,2} - x_2 \cdot \int (x_1 - t_1)_+ \, d\nu_{1,2=0}$$

$$- \int (x_1 - t_1)_+ (x_2 - t_2)_+ \, d\nu_{12}(t_1, t_2),$$

where $\nu_1, \nu_2, \nu_{1=0,2}, \nu_{1,2=0}$ are measures on $(0,1)$ and ν_{12} is a measure on $(0,1)^2$.

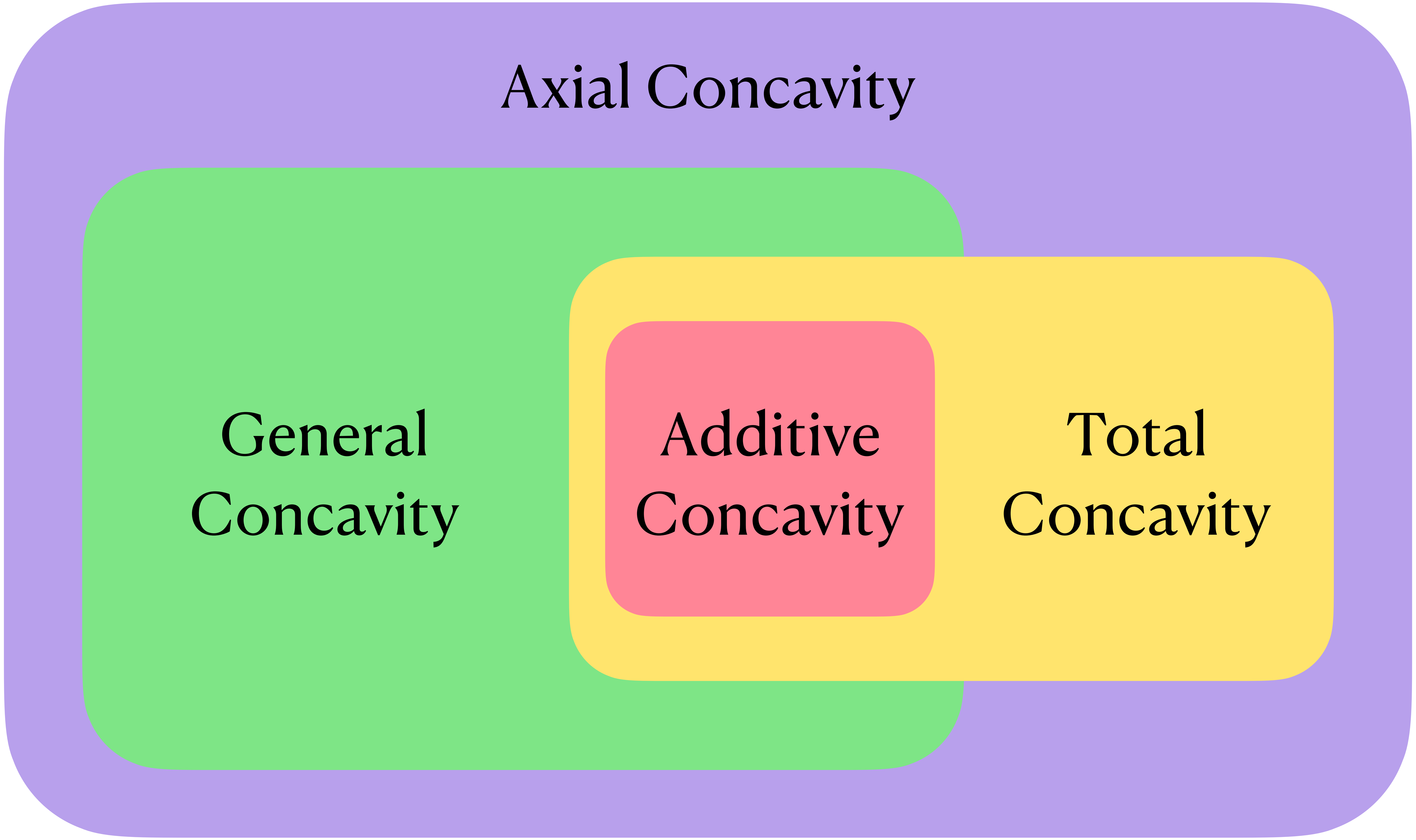
If f is a smooth totally concave function, then

$$\frac{\partial^2 f}{\partial x_1^2} \leq 0, \frac{\partial^2 f}{\partial x_2^2} \leq 0, \frac{\partial^3 f}{\partial x_1 x_2^2} \leq 0, \frac{\partial^3 f}{\partial x_1^2 x_2} \leq 0, \text{ and } \frac{\partial^4 f}{\partial x_1^2 x_2^2} \leq 0.$$

Characterization via Derivatives

- General Concavity: $\frac{\partial^2 f}{\partial x_1^2} \leq 0, \frac{\partial^2 f}{\partial x_2^2} \leq 0$, and $\left(\frac{\partial^2 f}{\partial x_1 x_2}\right)^2 \leq \frac{\partial^2 f}{\partial x_1^2} \cdot \frac{\partial^2 f}{\partial x_2^2}$.
- Axial Concavity: $\frac{\partial^2 f}{\partial x_1^2} \leq 0$ and $\frac{\partial^2 f}{\partial x_2^2} \leq 0$.
- Additive Concavity: $\frac{\partial^2 f}{\partial x_1^2} \leq 0, \frac{\partial^2 f}{\partial x_2^2} \leq 0$, and $\frac{\partial^2 f}{\partial x_1 x_2} = 0$.
- Total Concavity:

$$\frac{\partial^2 f}{\partial x_1^2} \leq 0, \frac{\partial^2 f}{\partial x_2^2} \leq 0, \frac{\partial^3 f}{\partial x_1 x_2^2} \leq 0, \frac{\partial^3 f}{\partial x_1^2 x_2} \leq 0, \text{ and } \frac{\partial^4 f}{\partial x_1^2 x_2^2} \leq 0.$$


Axial Concavity
General Concavity
Additive Concavity
Total Concavity

Extension to Higher Dimensions

Recall that when $d = 2$, f is totally concave if

$$\frac{\partial^2 f}{\partial x_1^2} \leq 0, \frac{\partial^2 f}{\partial x_2^2} \leq 0, \frac{\partial^3 f}{\partial x_1 x_2^2} \leq 0, \frac{\partial^3 f}{\partial x_1^2 x_2} \leq 0, \text{ and } \frac{\partial^4 f}{\partial x_1^2 x_2^2} \leq 0;$$

that is,

$$\frac{\partial^{p_1+p_2} f}{\partial x_1^{p_1} \partial x_2^{p_2}} \leq 0$$

for every $(p_1, p_2) \in \{0,1,2\}^2$ with $\max\{p_1, p_2\} = 2$.

For general d, f is totally concave if

$$\frac{\partial^{p_1+\cdots+p_d} f}{\partial x_1^{p_1} \cdots \partial x_d^{p_d}} \leq 0$$

for every $(p_1, \ldots, p_d) \in \{0,1,2\}^d$ with $\max_k p_k = 2$

Totally Concave Regression

Data: $(x^{(1)}, y_1), \ldots, (x^{(n)}, y_n)$ where $x^{(i)} \in [0,1]^d$ and $y_i \in \mathbb{R}$

$$\hat{f}_{\mathrm{TC}} \in \underset{f:\ \text{totally concave}}{\operatorname{argmin}} \sum_{i=1}^{n} \left(y_i - f(x^{(i)})\right)^2$$

It can be computed via finite-dimensional convex optimization algorithms.

Rate of Convergence

Under the standard set of model assumptions:

(1) $y_i = f^*(x^{(i)}) + \epsilon_i$ where f^* is totally concave and $\epsilon_i \overset{\text{i.i.d.}}{\sim} N(0, \sigma^2)$

(2) $x^{(1)}, \ldots, x^{(n)}$ form an equally-spaced lattice,

we have

multiplicative constant depends on d, σ, and f^*

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\left(\hat{f}_{\mathrm{TC}}(x^{(i)}) - f^*(x^{(i)})\right)^2\right] = O\left(n^{-\frac{4}{5}}(\log n)^{\frac{3(2d-1)}{5}}\right).$$

$\hat{f}_{TC}$ can avoid the curse of dimensionality to some extent.

Extensions

- We can restrict the order of interactions.

This leads to a faster rate of convergence.

- We can impose total concavity only on a subset of covariates.

The other covariates only appear via linear terms.

$$f(x_1, \ldots, x_d) = f_1(x_1, \ldots, x_p) + a_{p+1}x_{p+1} + \cdots + a_d x_d$$

where f_1 is a totally concave function and $a_{p+1}, \ldots, a_d \in \mathbb{R}$.

All of them are implemented in the R package regmdc, available at

https://github.com/DohyeongKi/regmdc.

Thank you for your attention!

https://arxiv.org/abs/2501.04360

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