

# **Smooth operator – using generalised additive models to quantify trends in noisy spatiotemporal data**

Gavin Simpson

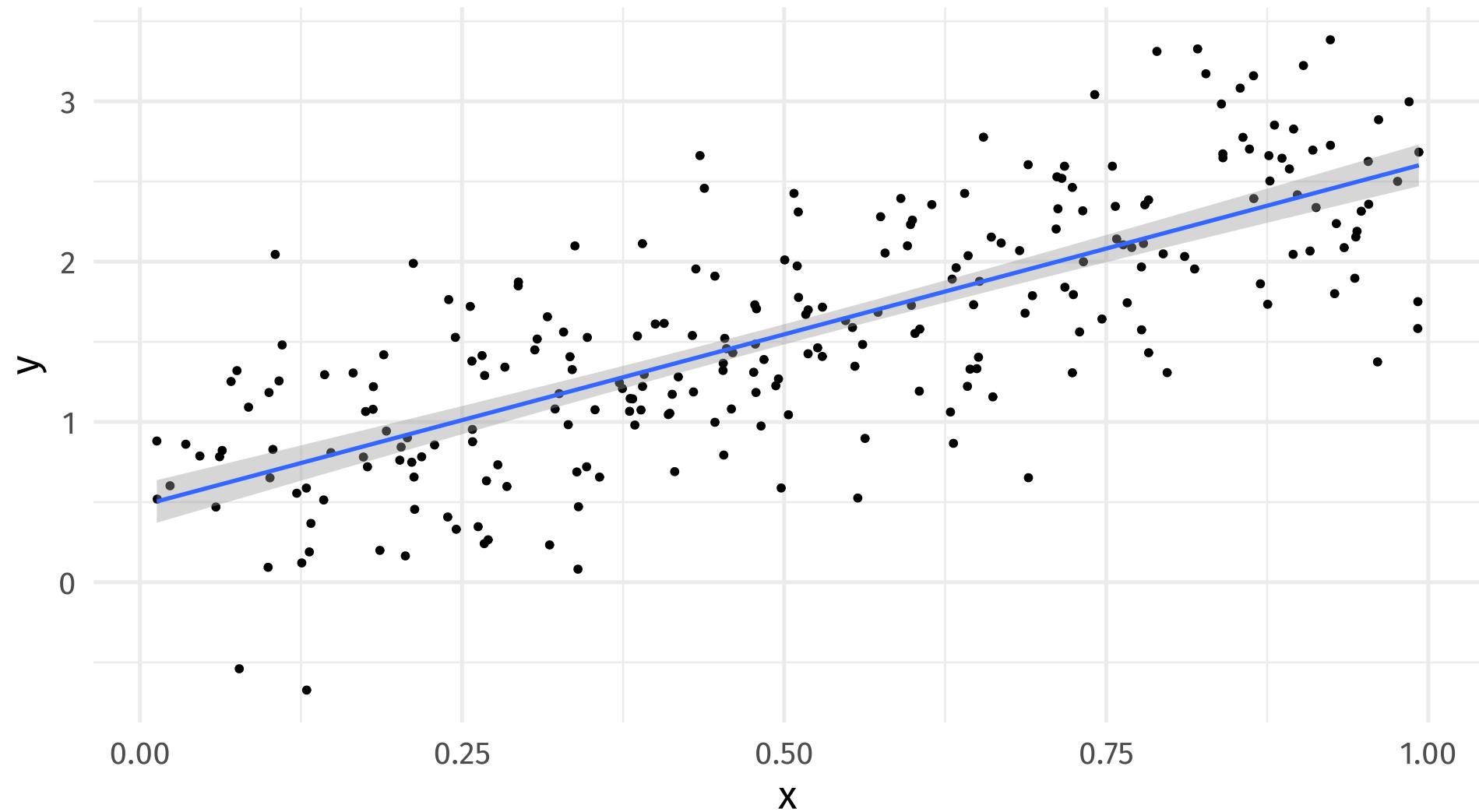
HIFMB · University of Oldenburg · November 3, 2020

**Use statistics to learn from  
data in presence of noise**



Data has a better idea

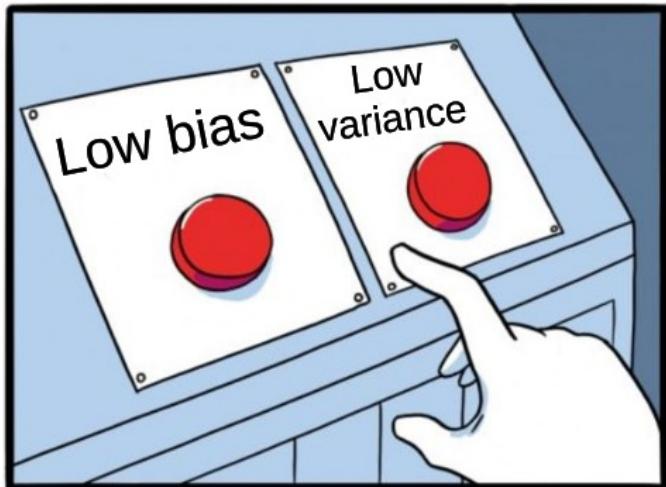
# Learning from data



# DEEP LEARNING

## STATISTICS TURNED UP TO ELEVEN

# Learning involves trade-offs



# Generalized Additive Models

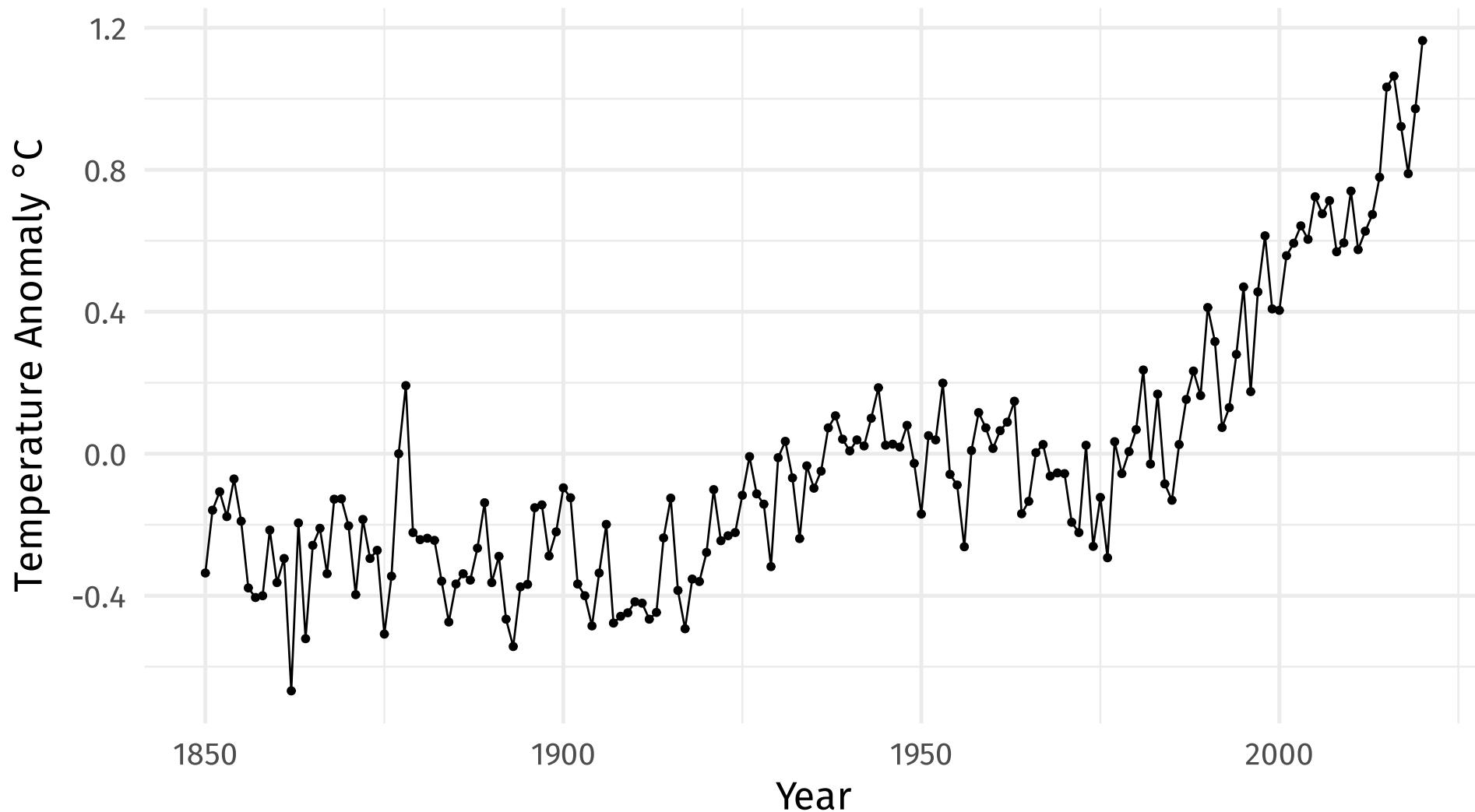
Linear Models

GAMs

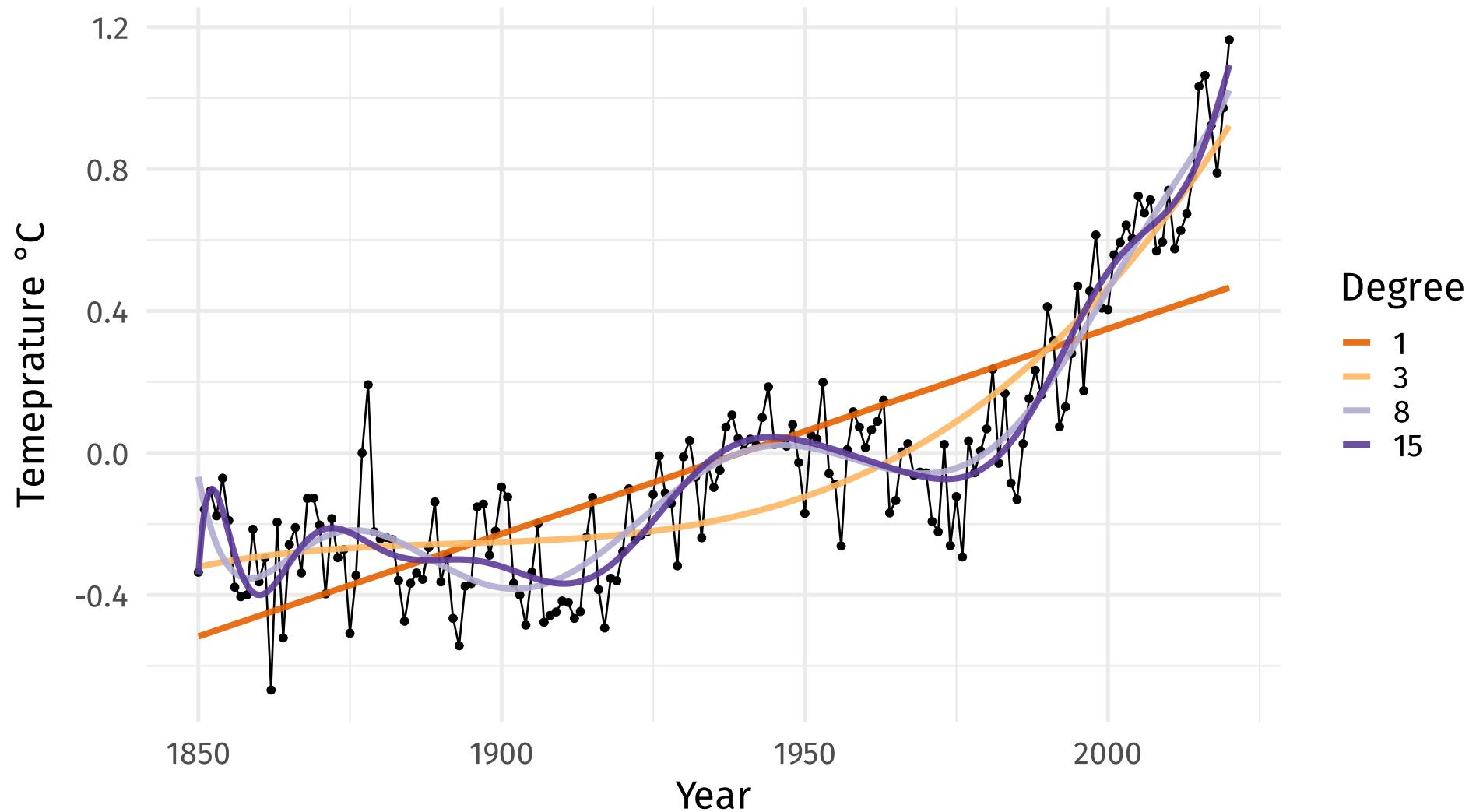
Black-Box ML



# HadCRUT4 time series

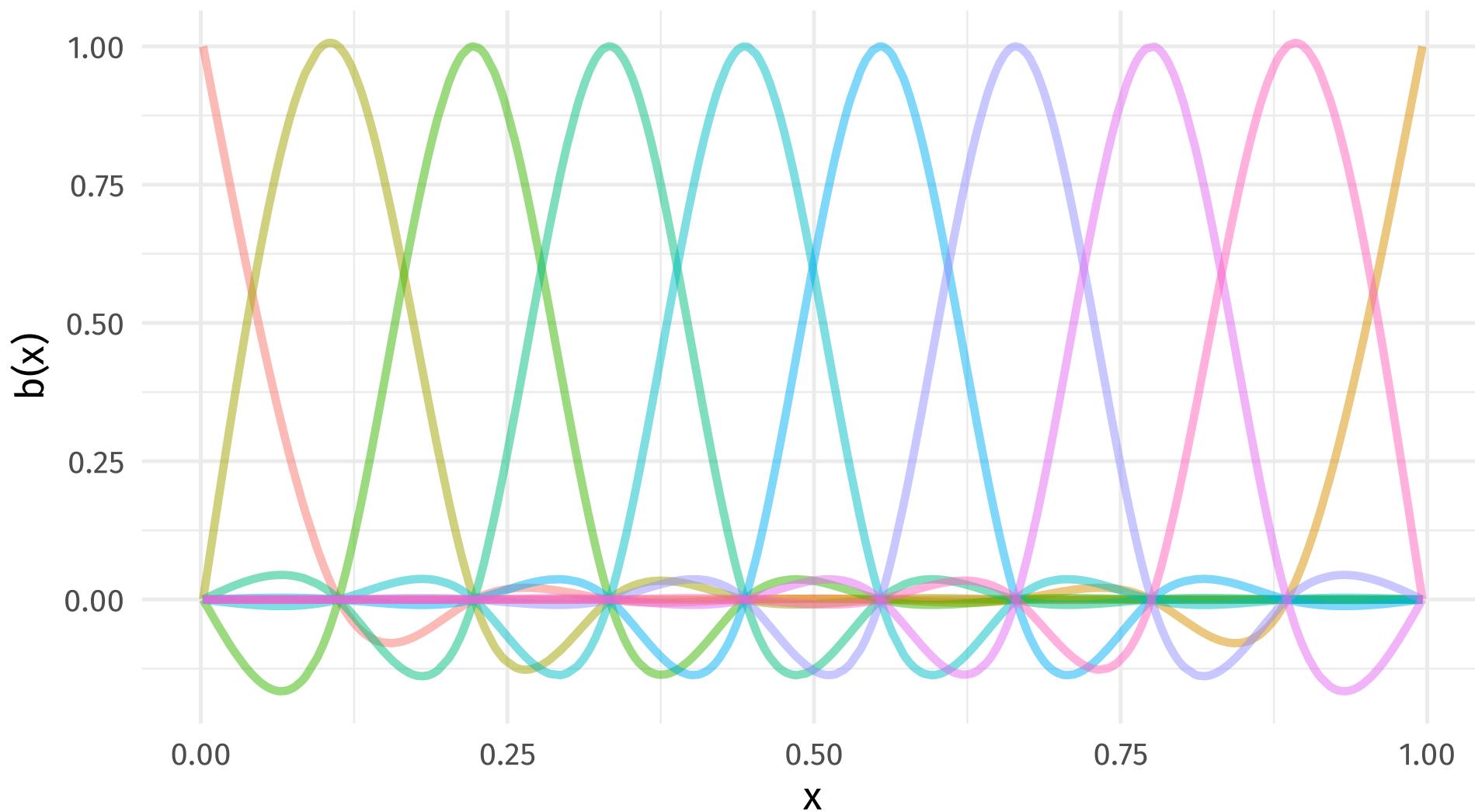


# Polynomials

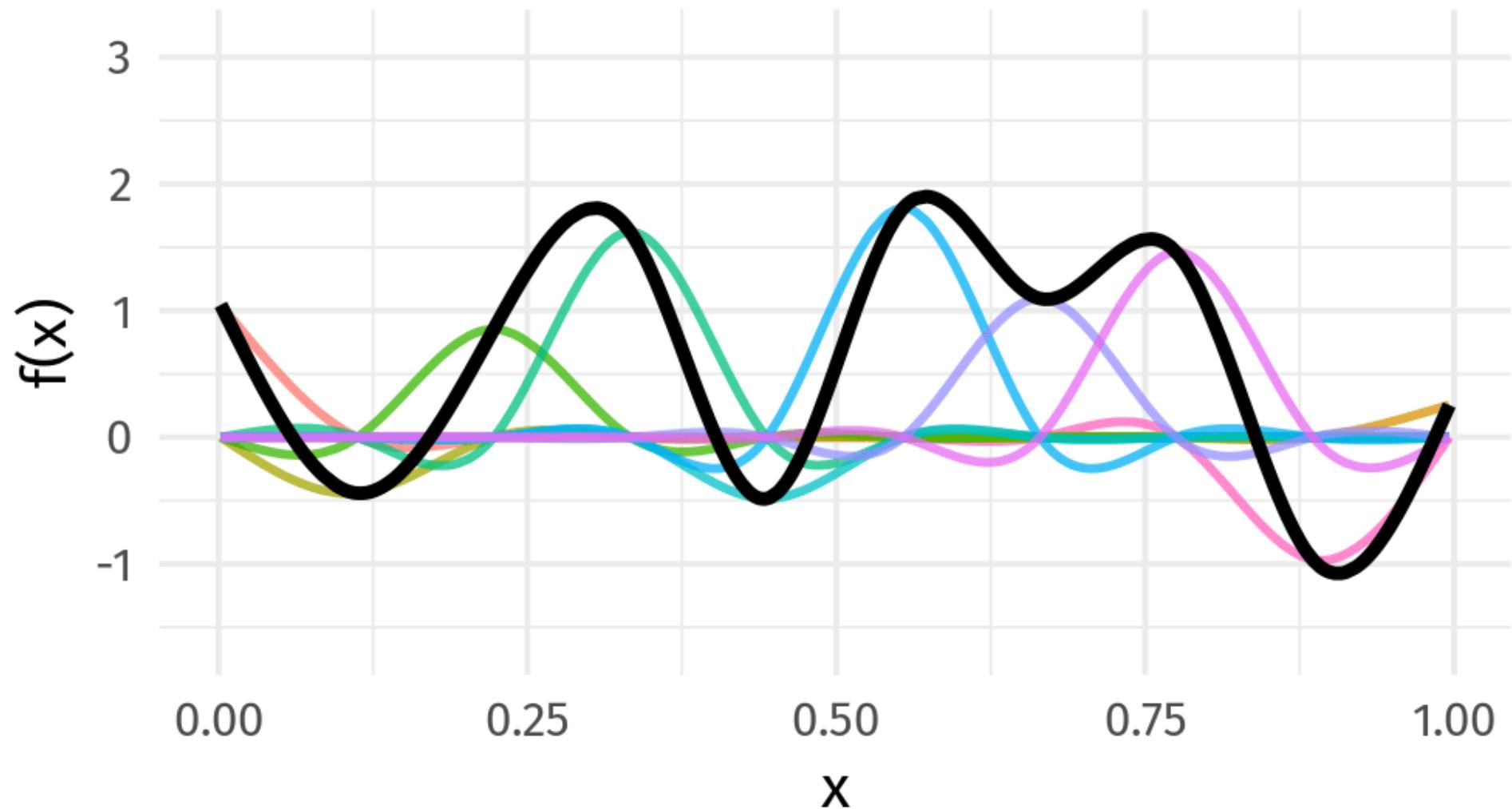


# GAMs use splines

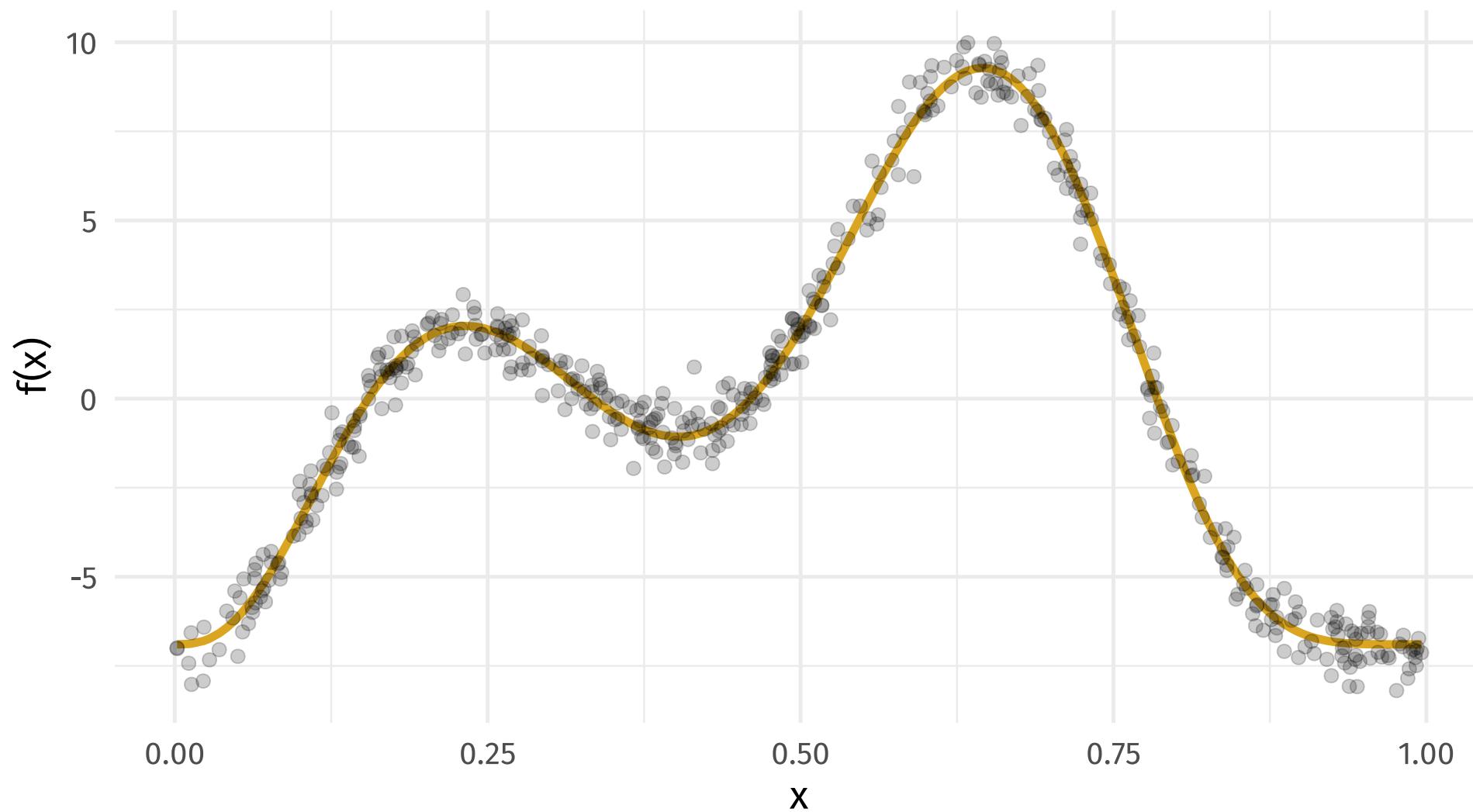
# Splines formed from basis functions



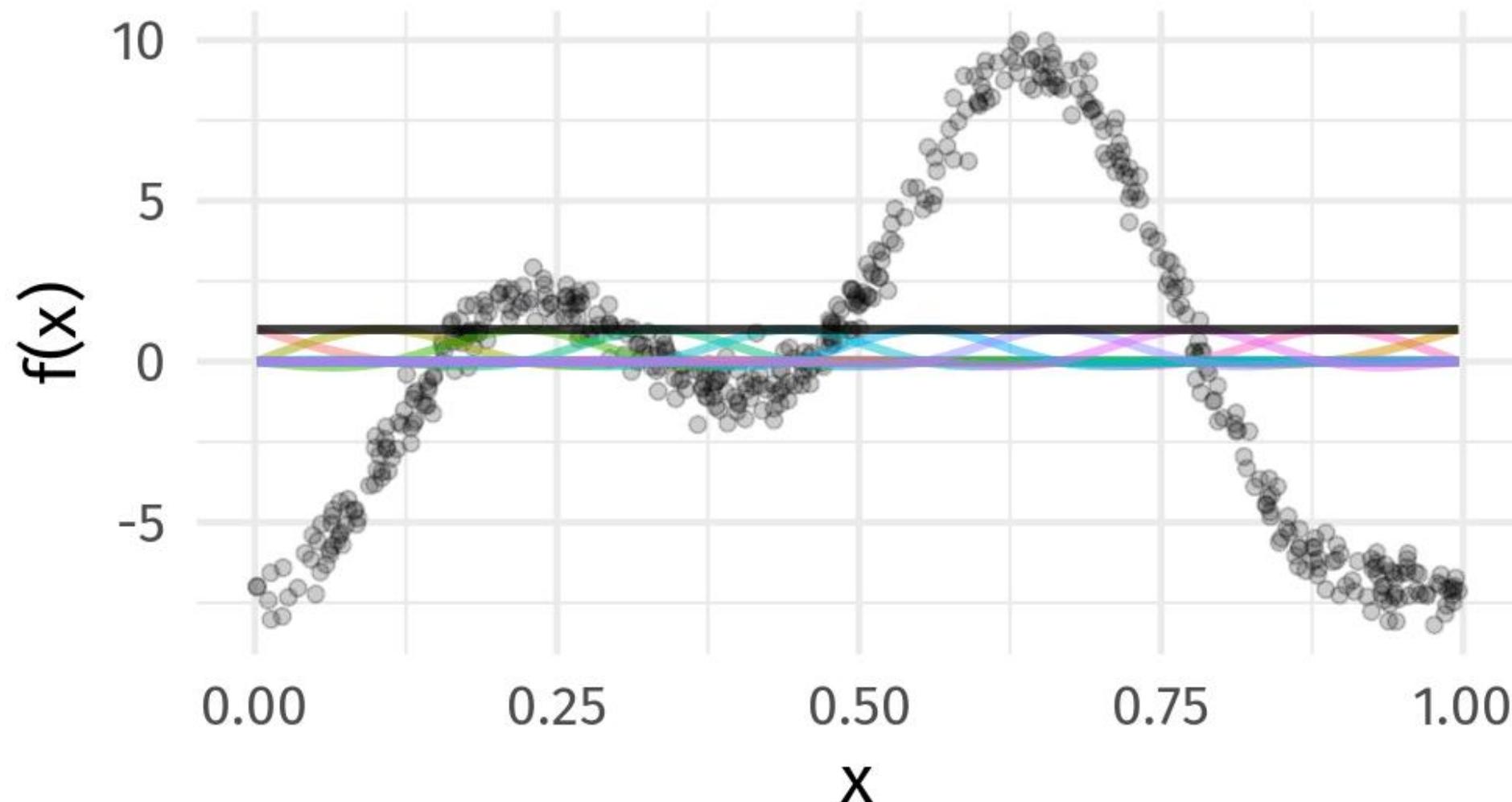
# Weight basis functions $\Rightarrow$ spline



# How do GAMs learn from data?



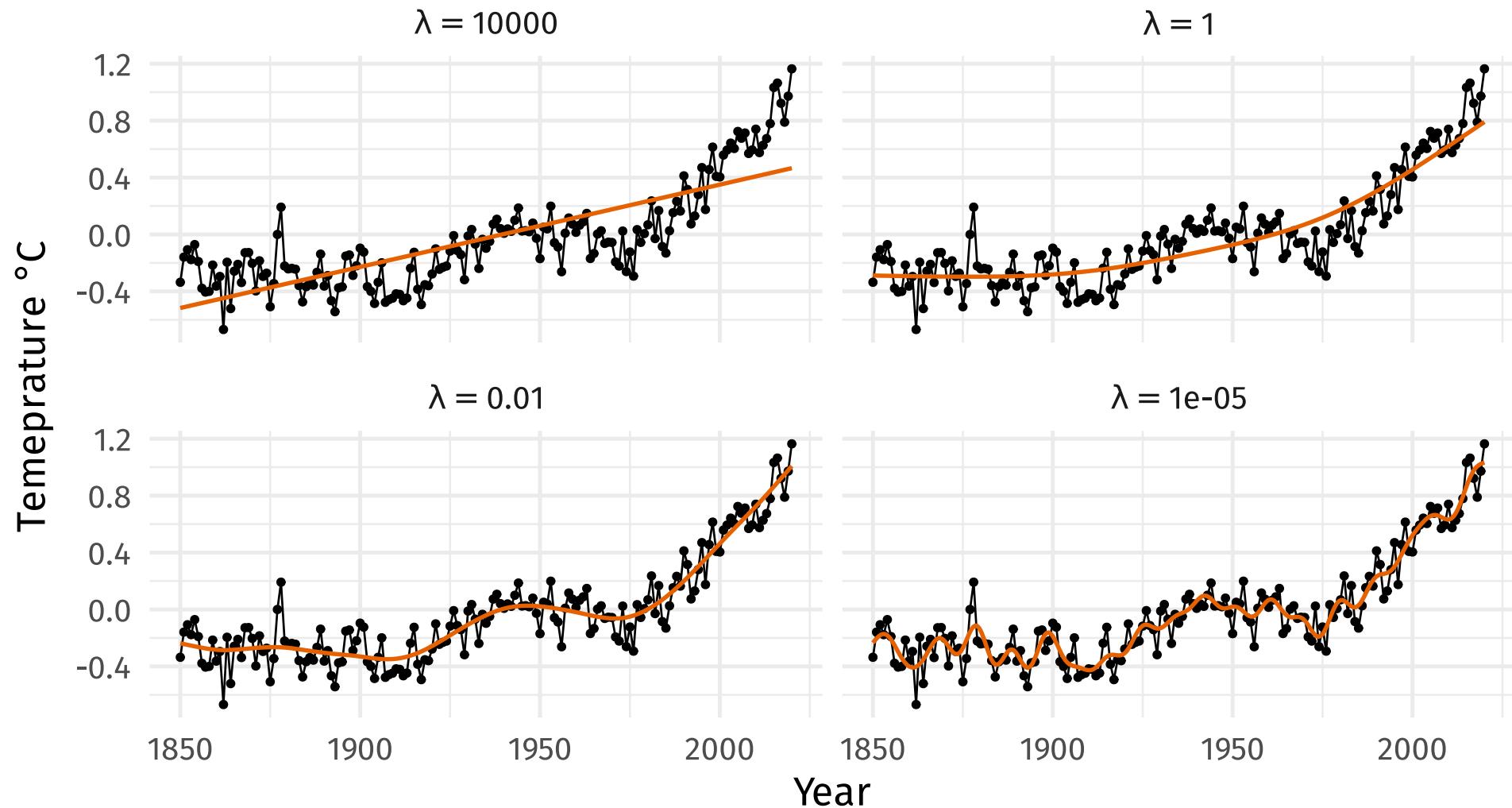
# Maximise penalised log-likelihood $\Rightarrow \beta$



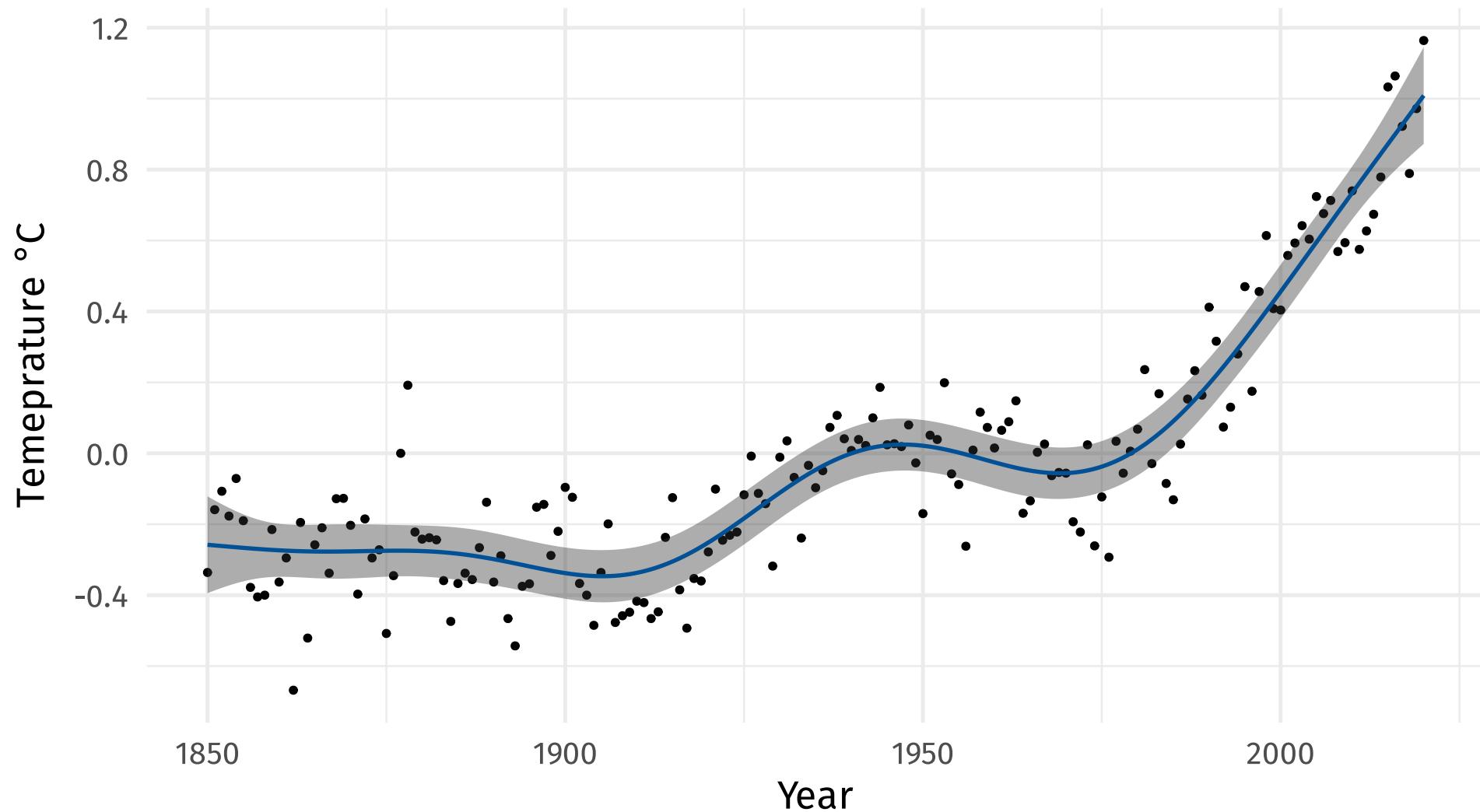
# Avoid overfitting our sample

**Use a wiggliness penalty –  
avoid fitting too wiggly models**

# HadCRUT4 time series



# Fitted GAM



# vignettes

# Vignette 1

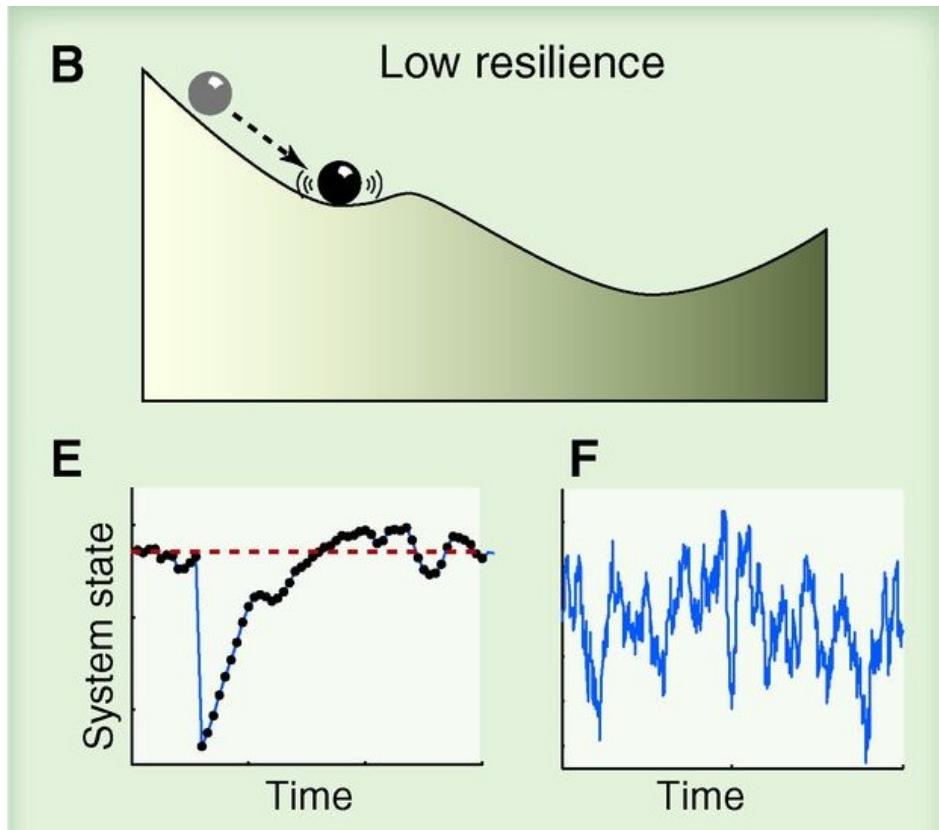
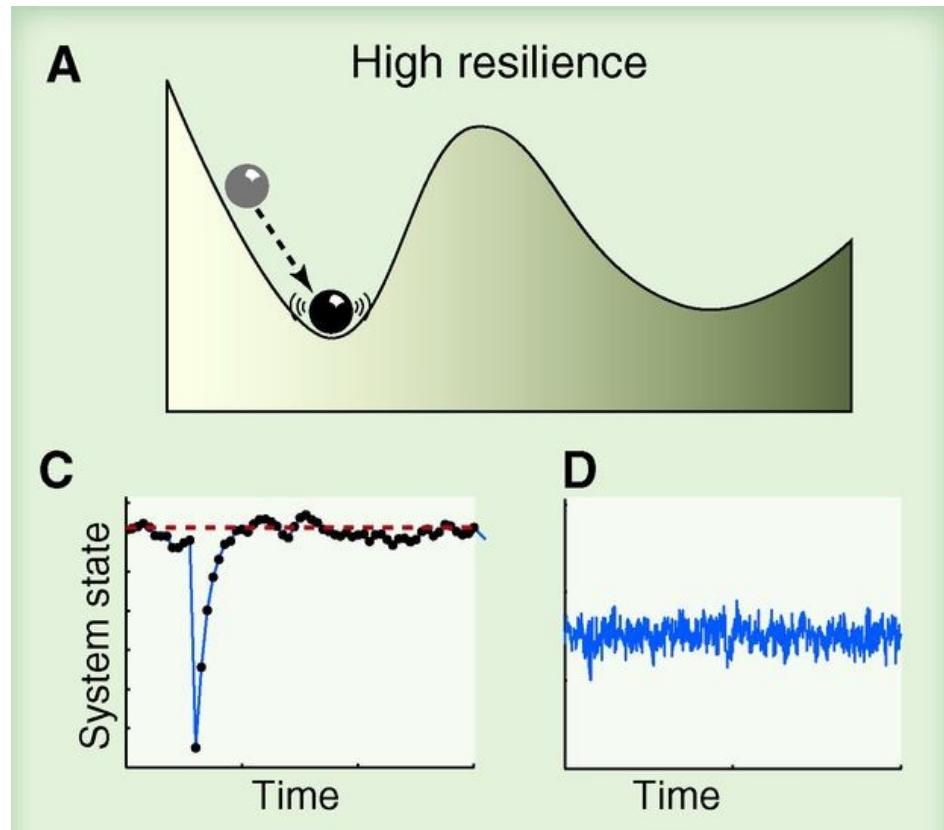
# **Statistical estimation of ecosystem variance**

# Mean

# Variance

# Variance

Intuitive & key descriptor of ecosystem state

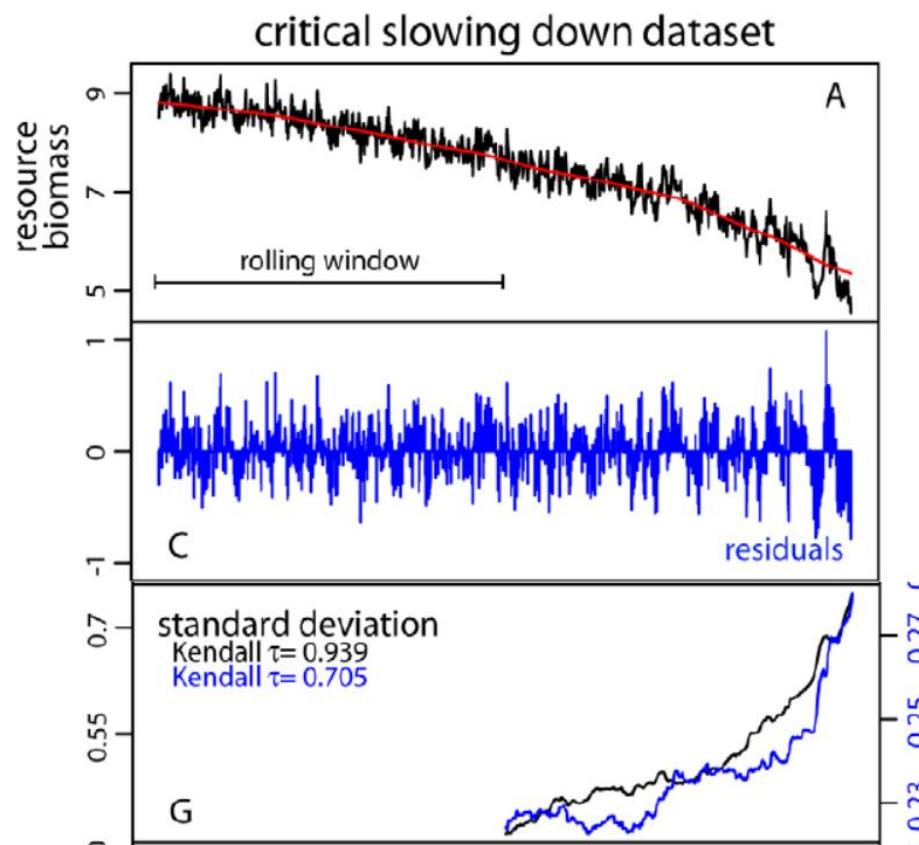


Source: Scheffer *et al* Science (2012)

# Moving windows – don't do this!

Moving window approach:

1. detrend
2. choose window size
3. estimate variance
4. move window 1 time step
5. repeat 3. & 4. until done
6. look for trend



Modified from Dakos *et al* (2012) PLOS One

# Problems

*Ad hoc*

- How to detrend (method, complexity of trend, ...)
- What window width?

Ideally regularly spaced data

- What to do about gaps, missing data, irregularly spaced data?

Statistical testing hard

- Kendall's  $\tau$  assumes independence
- Surrogate time series assumes regular sampling, sensitive to choice of ARMA

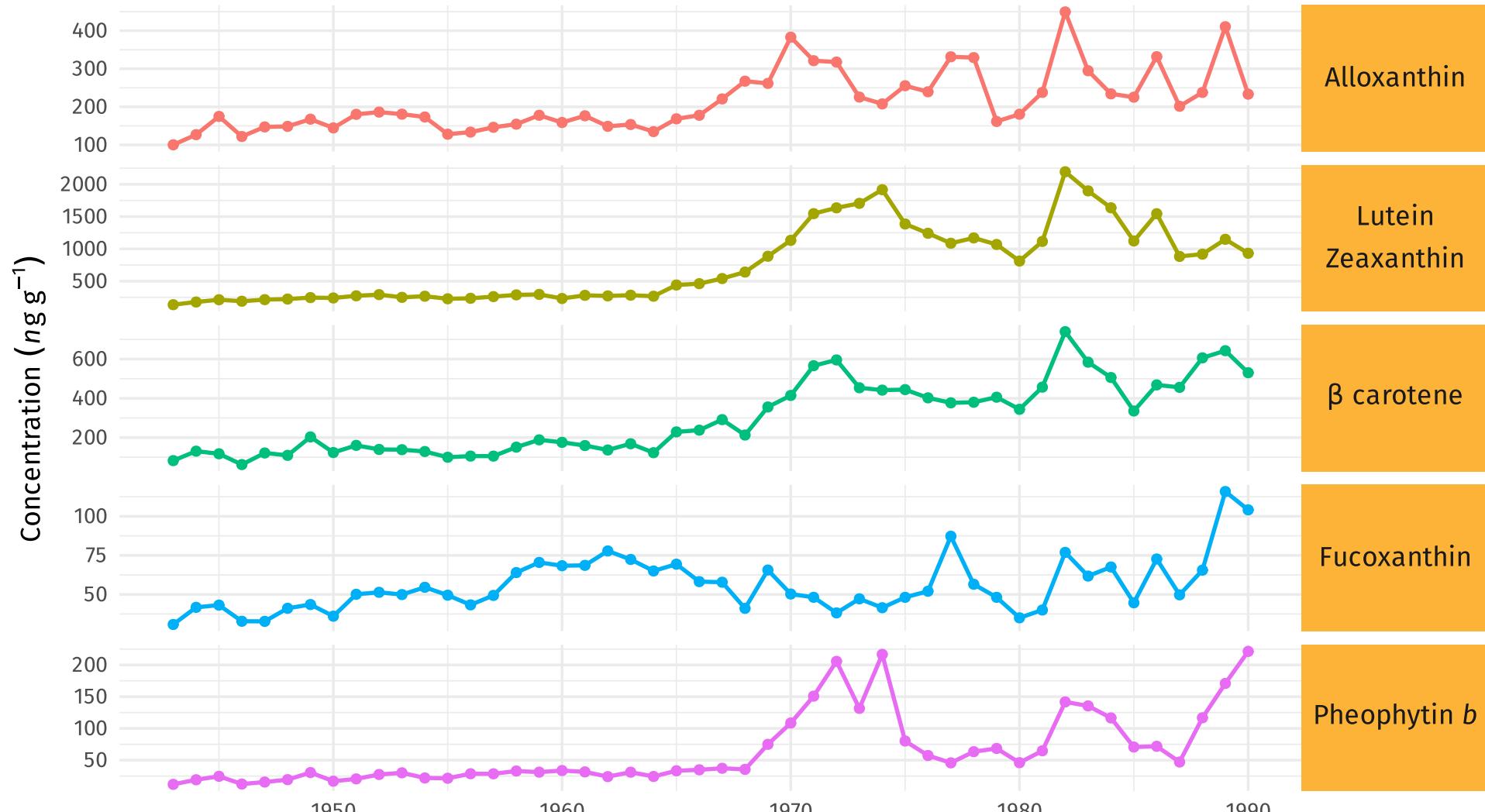
Lake 227

# Lake 227

- Experimentally manipulated
- Annual sediment samples 1943–1990
- Analyzed for fossil pigments

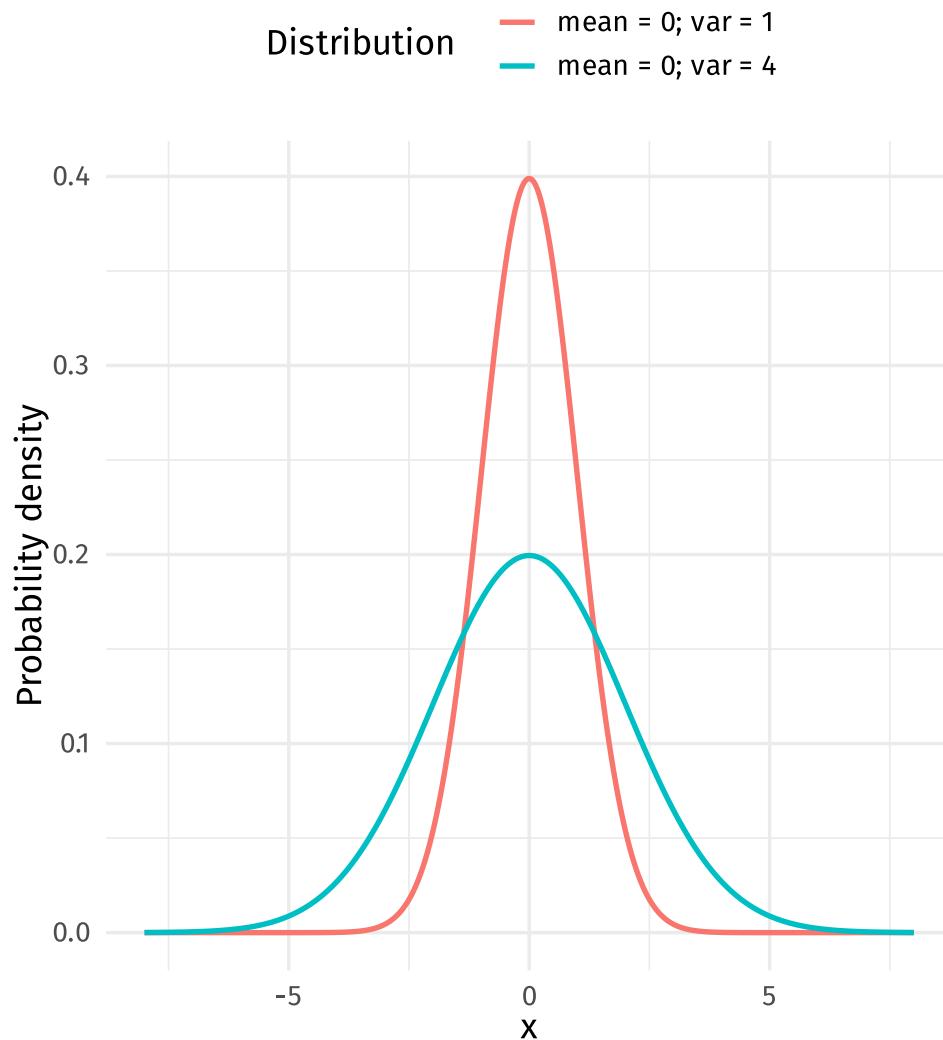
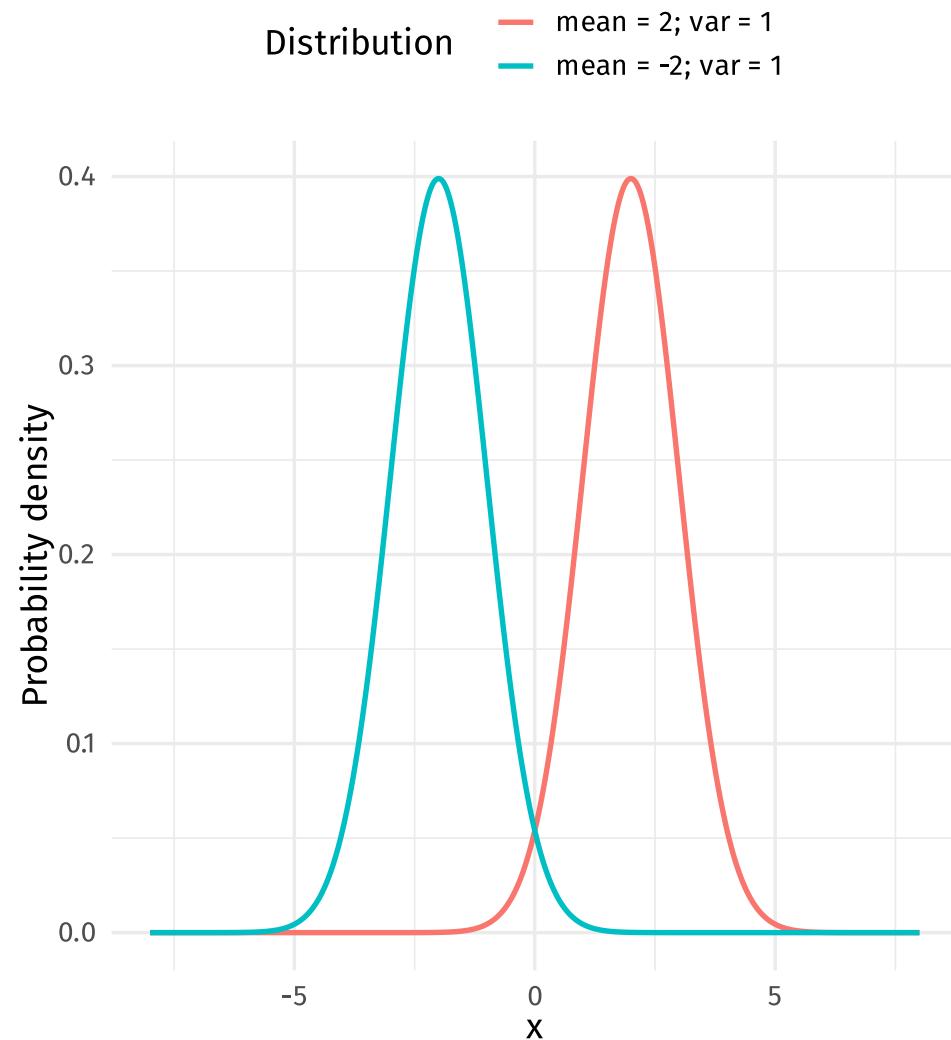
Cottingham *et al* (2000) **Ecology Letters** showed via a Levene's test that **variances** pre- & post-intervention were different

# Lake 227



# Challenge

# Parameters beyond the mean



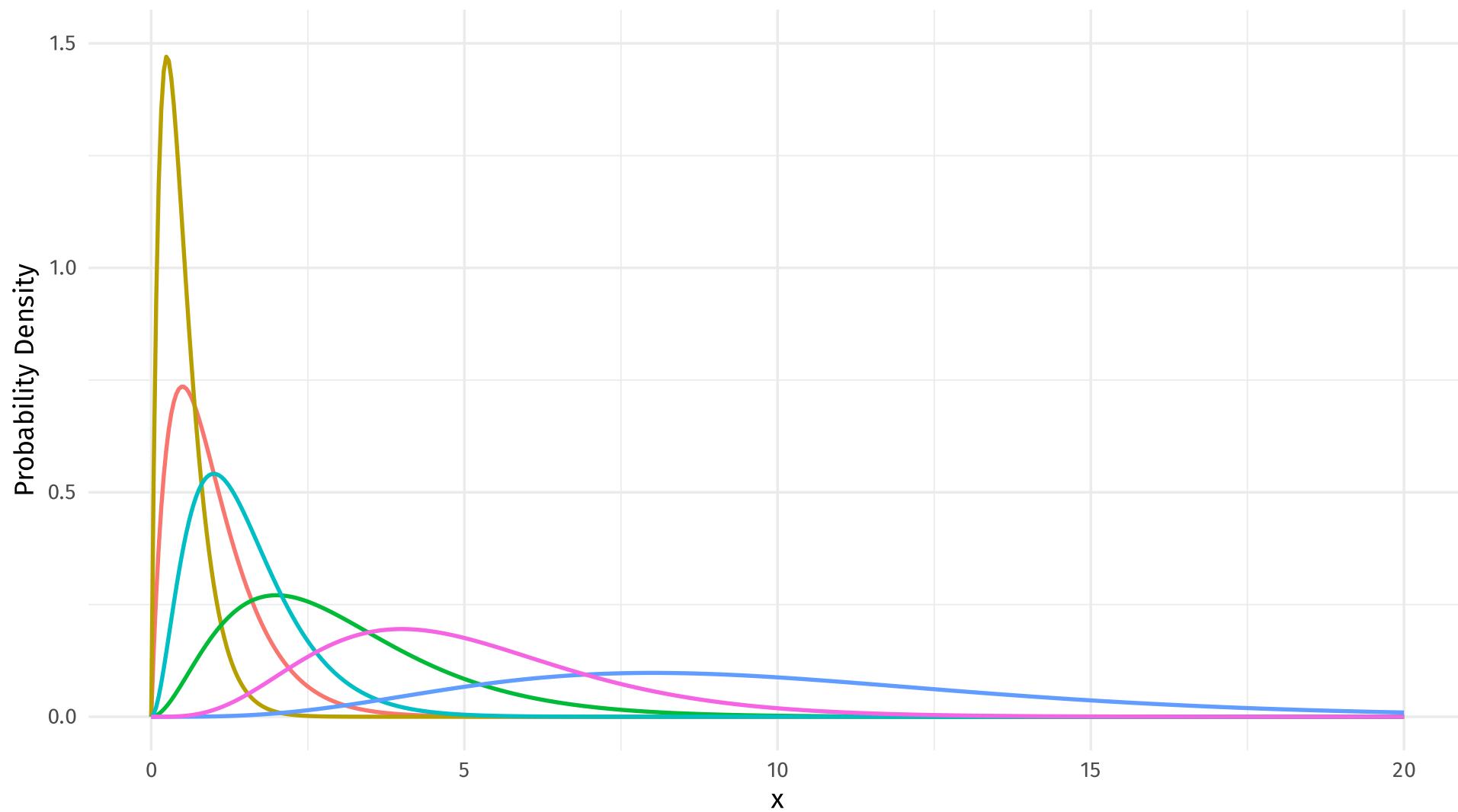
# Distributional models

$$y_i | \boldsymbol{x}_i \sim \mathcal{D}(\vartheta_1(\boldsymbol{x}_i), \dots, \vartheta_K(\boldsymbol{x}_i))$$

For the Gaussian distribution

- $\vartheta_1(\boldsymbol{x}_i) = \mu(\boldsymbol{x}_i)$
- $\vartheta_2(\boldsymbol{x}_i) = \sigma(\boldsymbol{x}_i)$

# The Gamma distribution



# Lake 227 sedimentary pigments

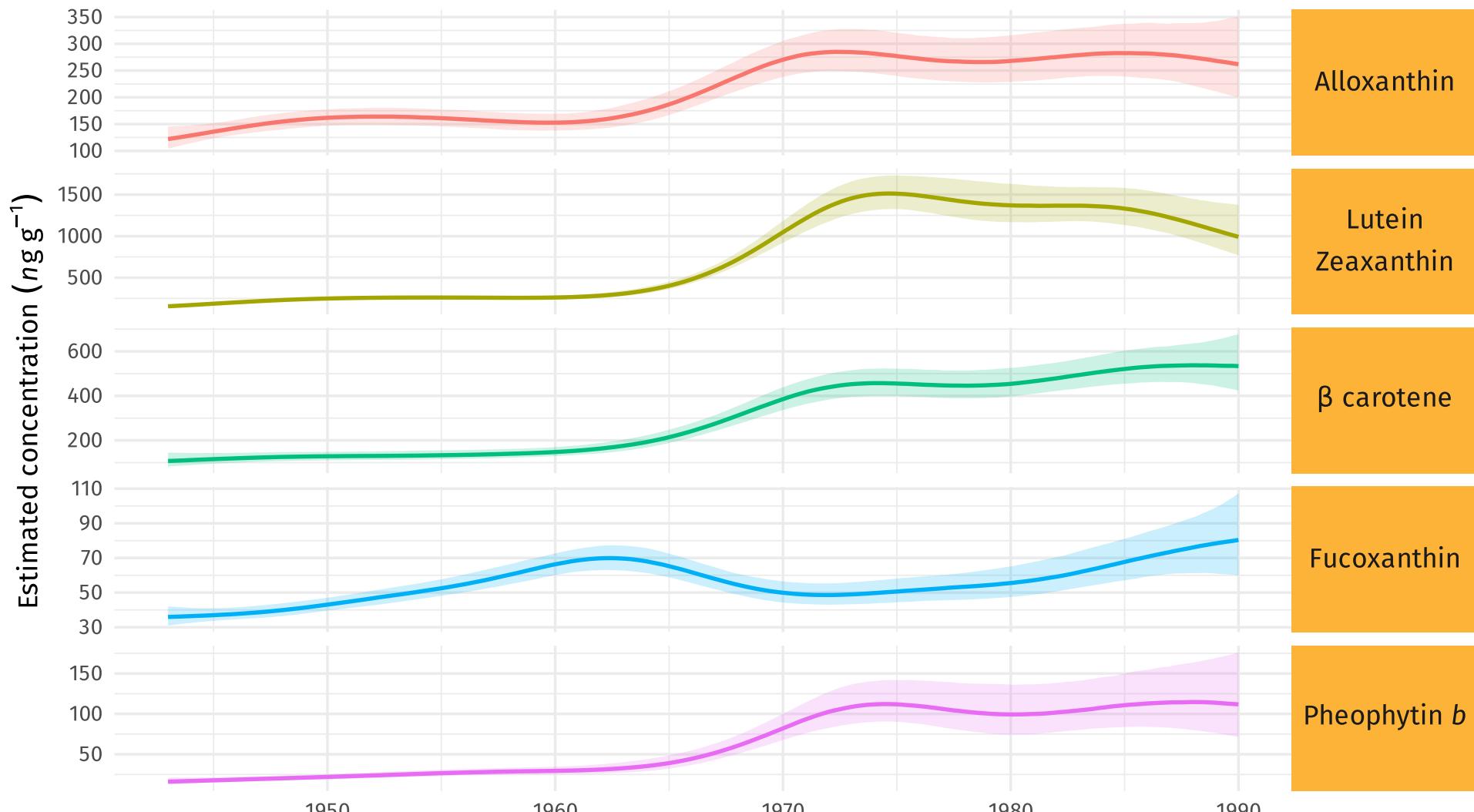
Fitted gamma distributional model using **brms** and **Stan**

$$y_t \sim \mathcal{G}(\mu = \eta_{1,t}, \alpha = \eta_{2,t})$$

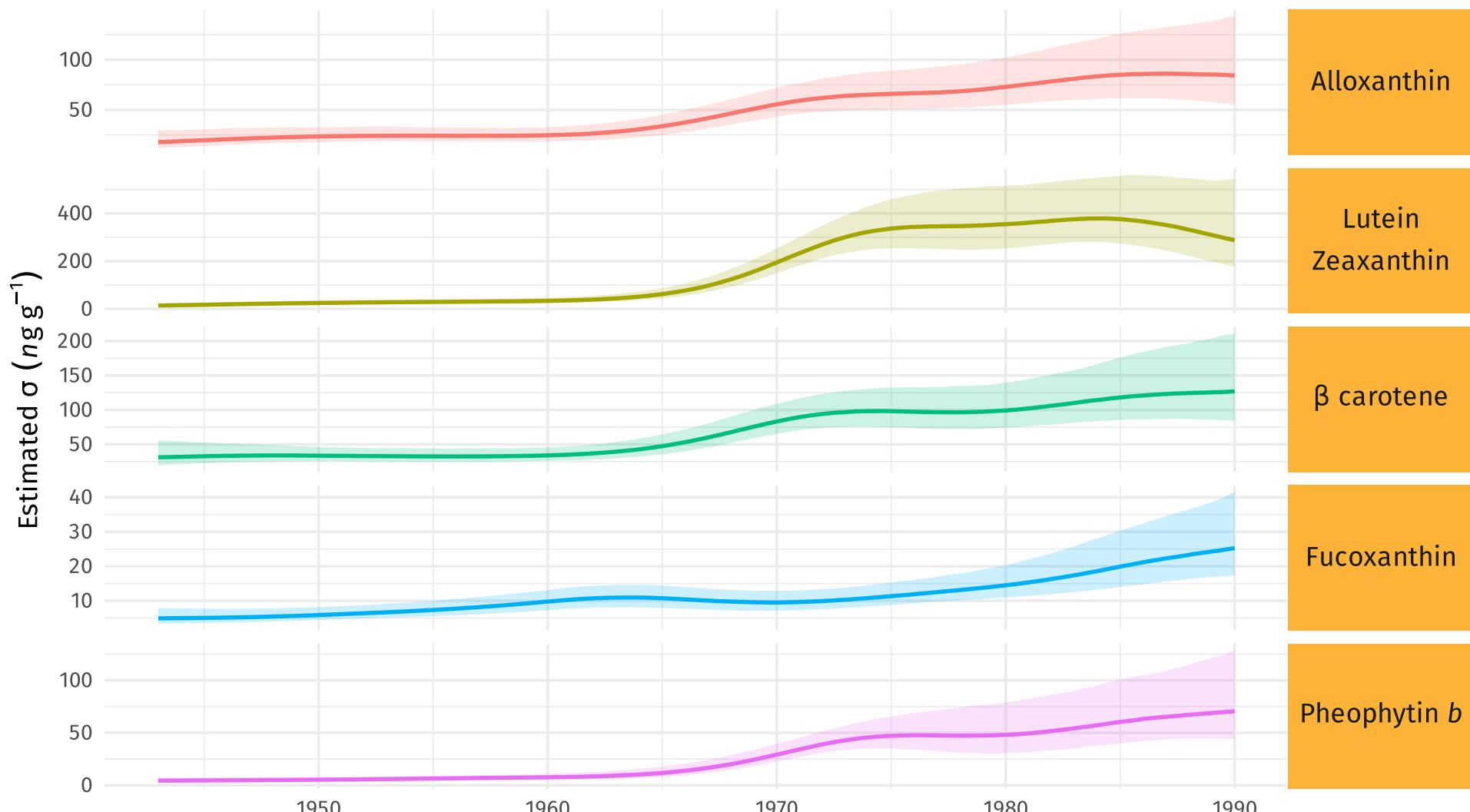
$$\eta_{1,t} = \exp(f_{1,\text{pigment}}(\text{Year}_t))$$

$$\eta_{2,t} = \exp(f_{2,\text{pigment}}(\text{Year}_t))$$

# Results – pigment means



# Results – pigment variances



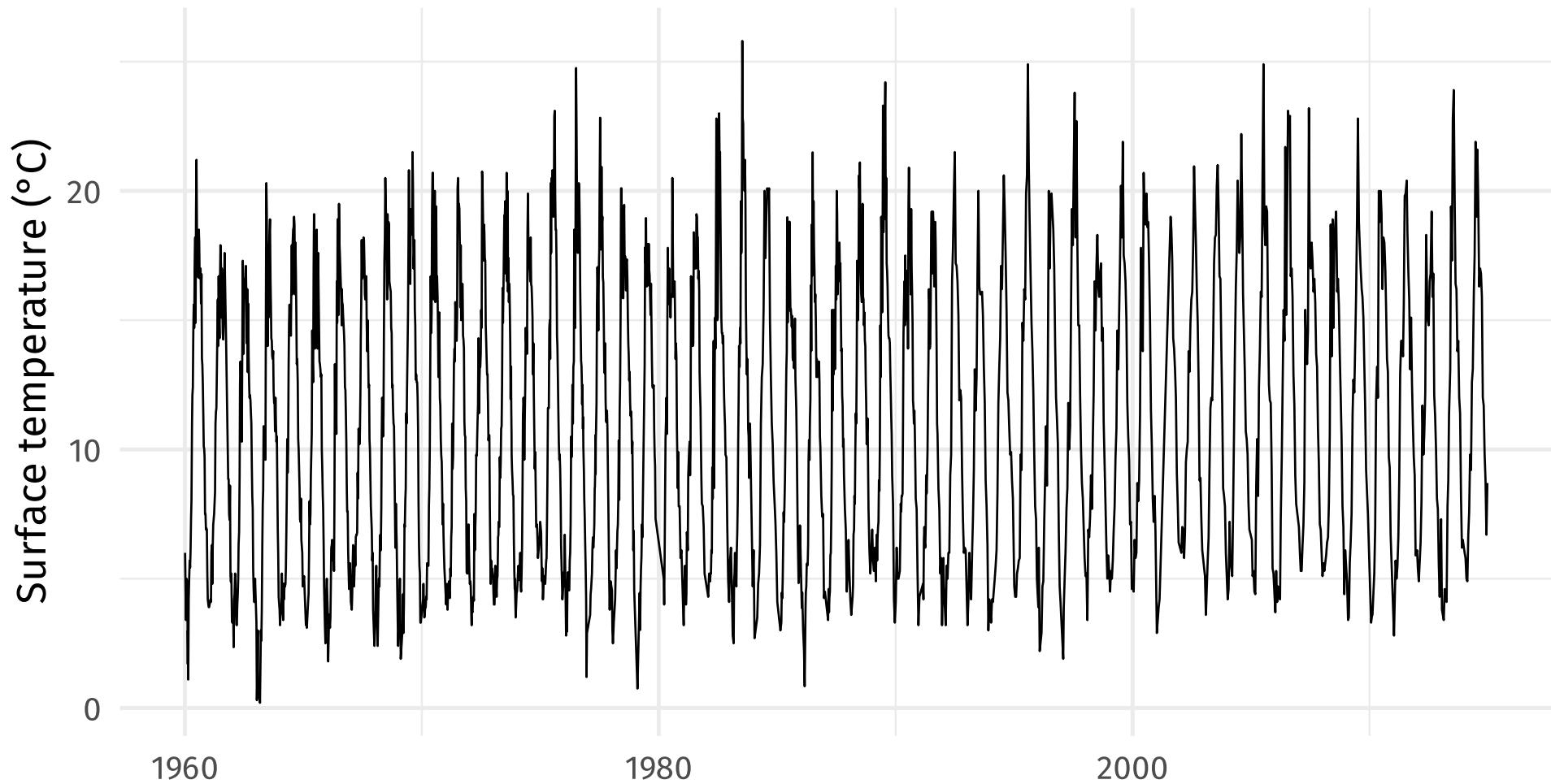
# Summary

- Using distributional GAMs we now have a means to robustly estimate the variance of a system and how that variance changes over time
- Use models such as these to begin to quantify an important ecological metric from a principled statistical view point

# Vignette 2

**Climate change affecting lake  
temperatures?**

# Blelham Tarn, UK



Data: Woolway *et al* (2019) *Climate Change* **155**, 81–94 [doi: 10/c7z9](https://doi.org/10/c7z9)

**Why worry about minimum  
temperatures?**

# Why worry about minimum temperatures?

Annual minimum temperature is a strong control on many in-lake processes (eg Hampton *et al* 2017)

Extreme events can have long-lasting effects on lake ecology – mild winter in Europe 2006–7 (eg Straile *et al* 2010)

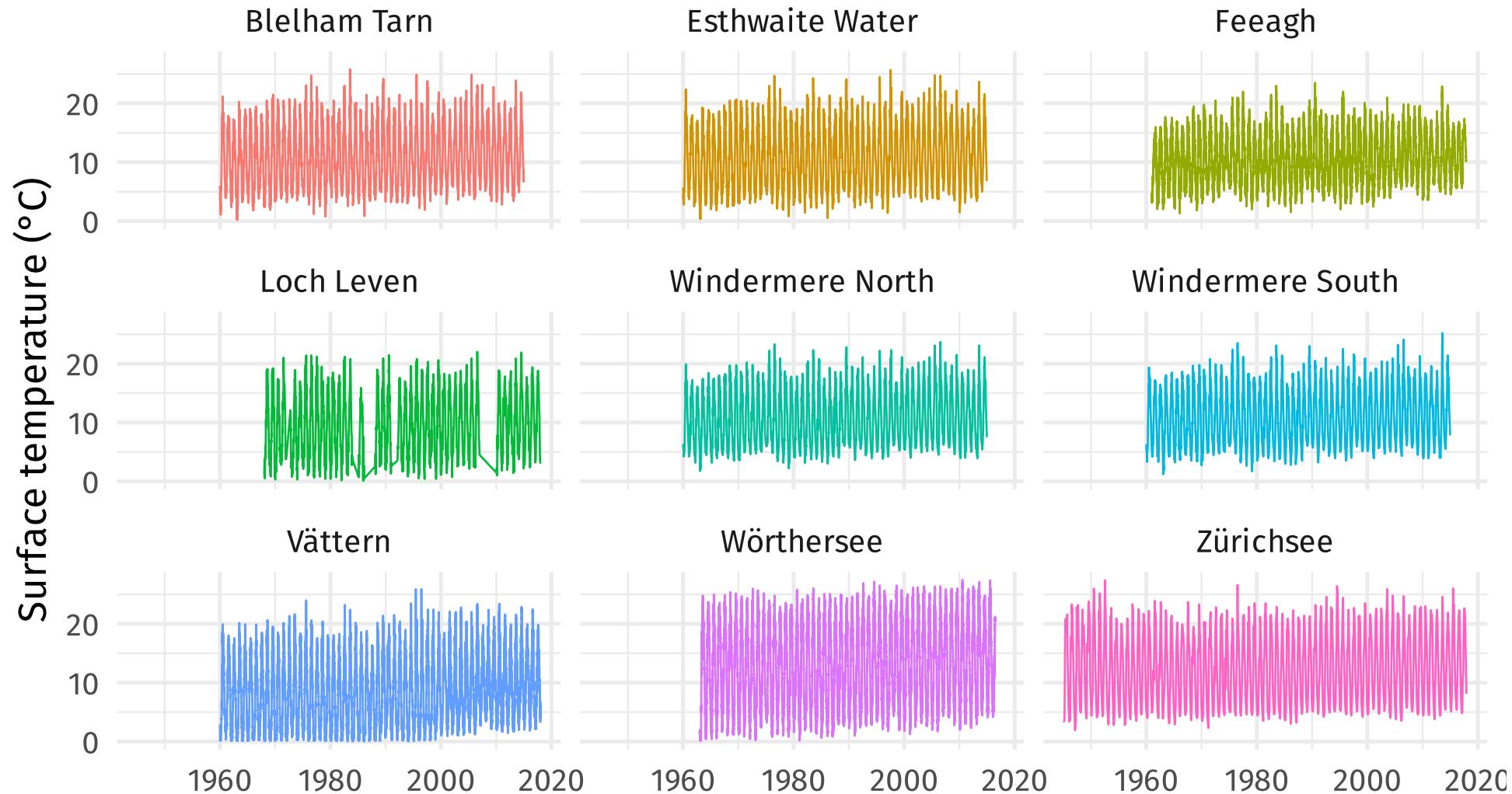
Reduction in habitat or refugia for cold-adapted species

- Arctic charr (*Salvelinus alpinus*)
- Opossum shrimp (*Mysis salemaai*)

Hampton *et al* (2017). Ecology under lake ice. *Ecology Letters* **20**, 98–111. [doi: 10/f3tpzh](https://doi.org/10/f3tpzh)

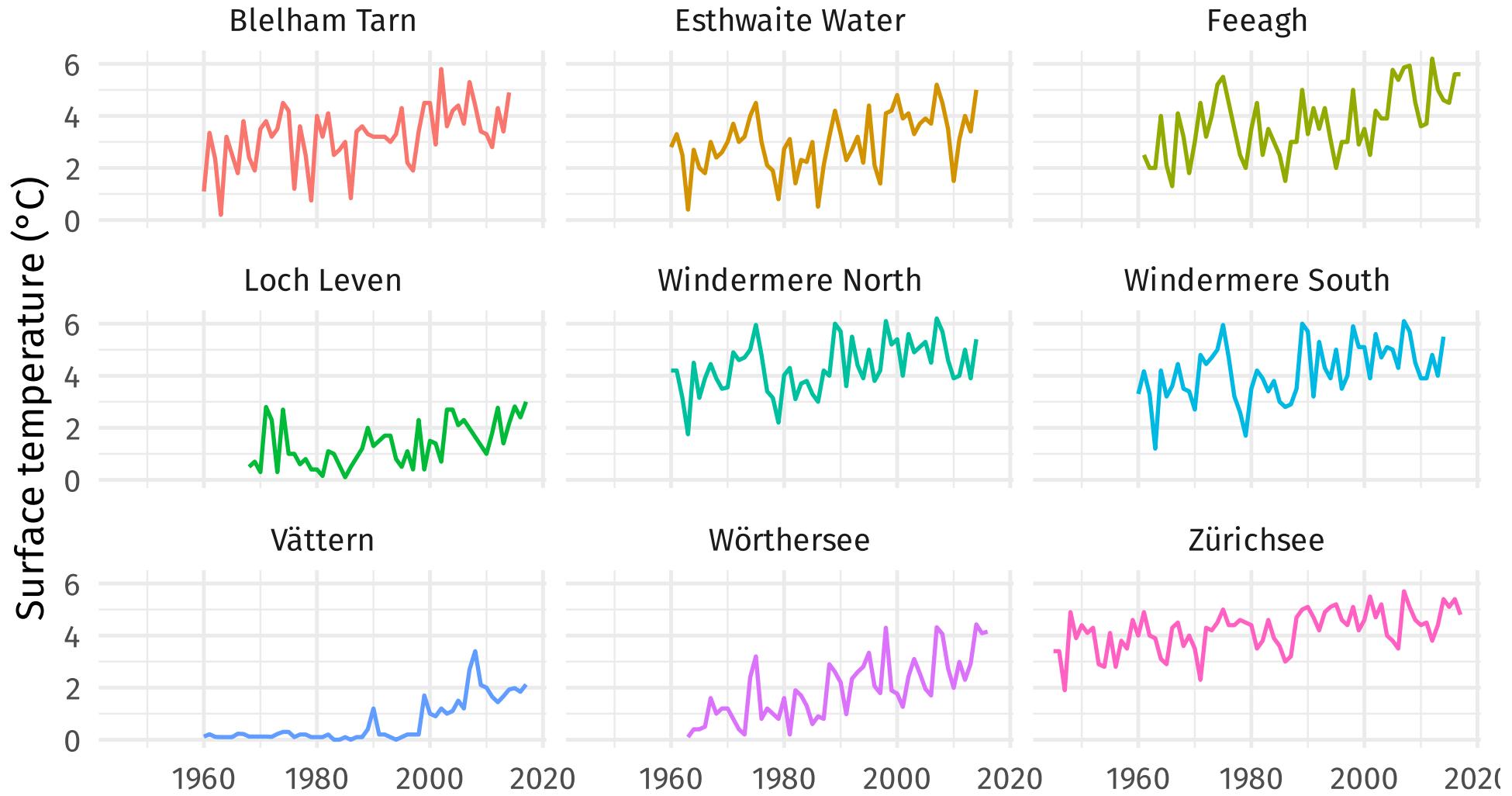
Straile *et al* (2010). Effects of a half a millennium winter on a deep lake – a shape of things to come? *Global Change Biology* **16**, 2844–2856. [doi: 10/bx6t4d](https://doi.org/10/bx6t4d)

# Multiple time series $\Rightarrow$ HGAM



# Central Limit Theorem

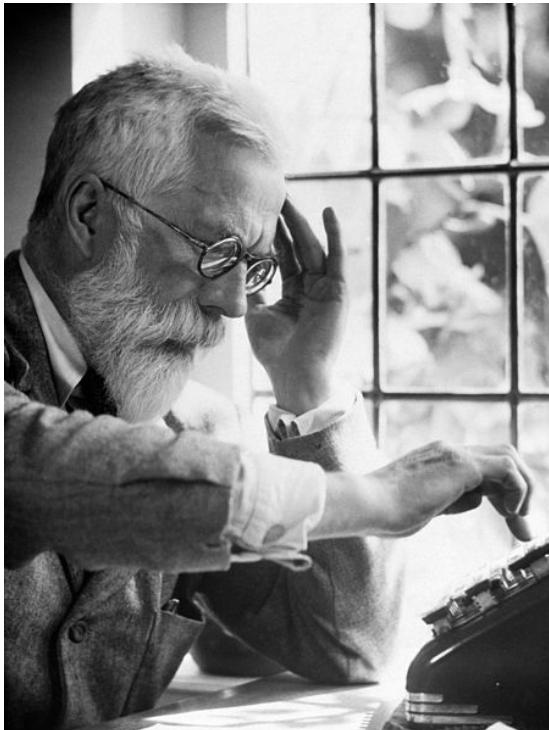
# Annual minimum temperature



# Block Minima

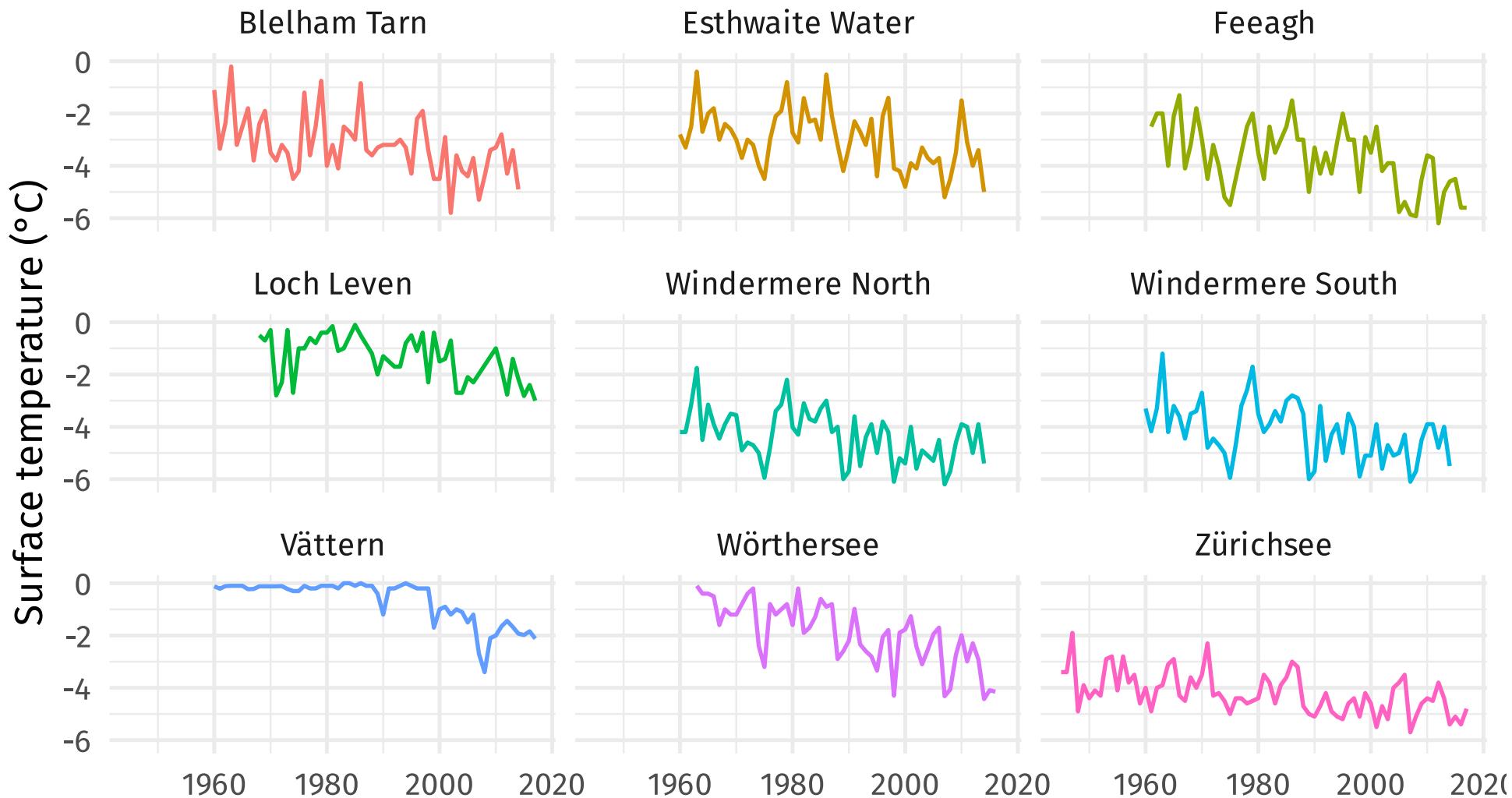
# Fisher–Tippett–Gnedenko theorem

The **maximum** of a sample of  $iid$  random variables after proper renormalization can only converge in distribution to one of three possible distributions; the *Gumbel* distribution, the *Fréchet* distribution, or the *Weibull* distribution.



**Block Minima...?**

# Negate the minima $\Rightarrow$ maxima



**Three  
Distributions...?**

# Generalised extreme value distribution

In 1978 Daniel McFadden demonstrated the common functional form for all three distributions – the GEVD

$$G(y) = \exp\left\{ -\left[ 1 + \xi \left( \frac{y - \mu}{\sigma} \right) \right]_+^{-1/\xi} \right\}$$

Three parameters to estimate

- location  $\mu$ ,
- scale  $\sigma$ , and
- shape  $\xi$

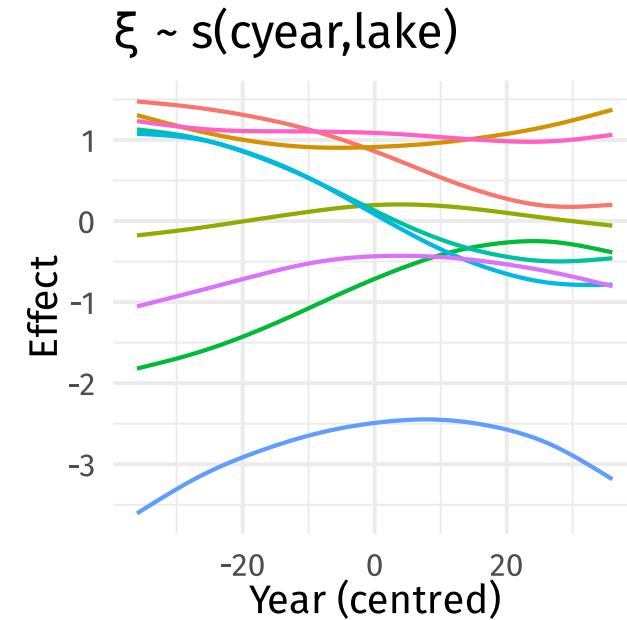
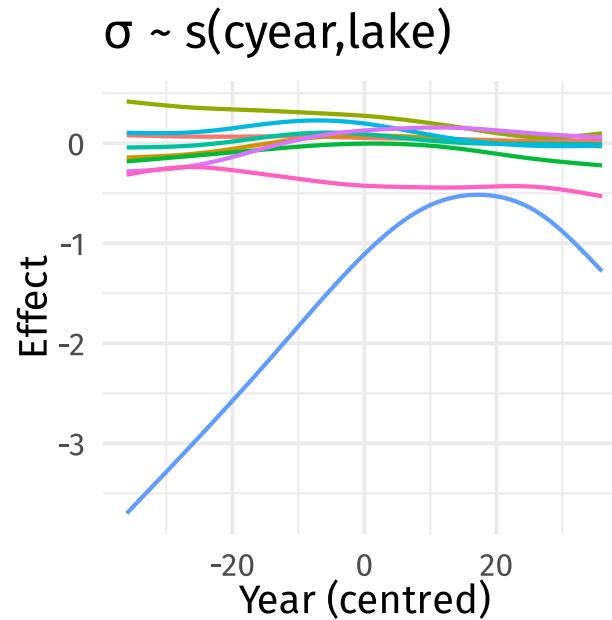
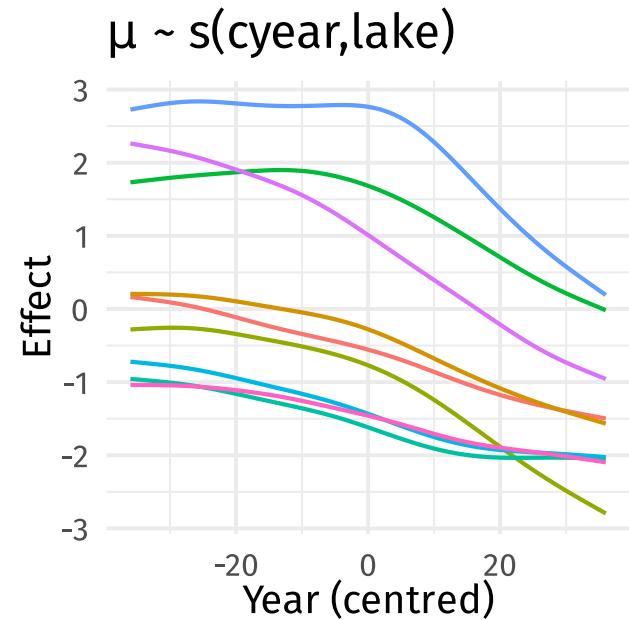
Three distributions

- Gumbel distribution when  $\xi = 0$ ,
- Fréchet distribution when  $\xi > 0$ , &
- Weibull distribution when  $\xi < 0$

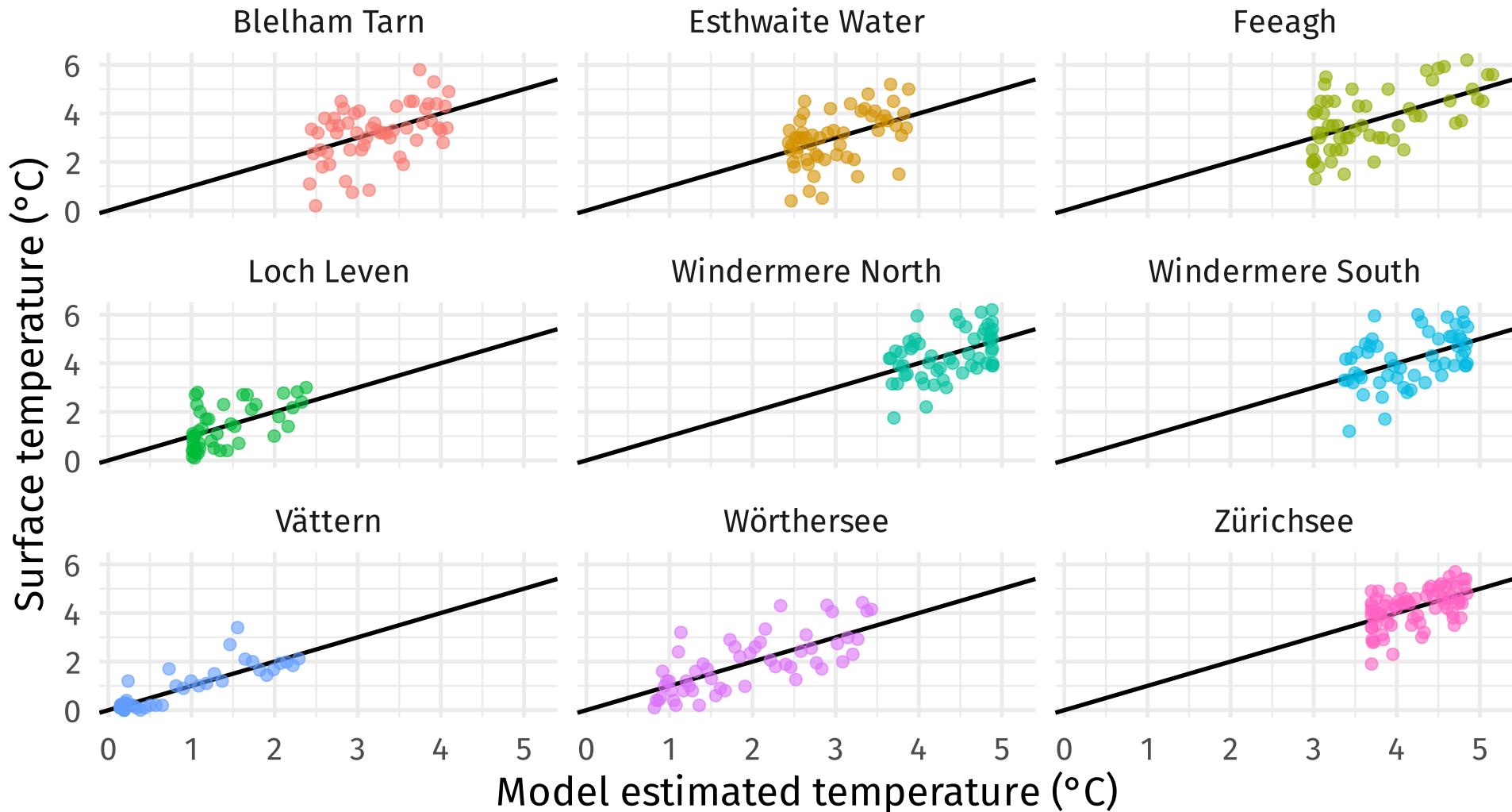
**Fit Distributional GAM using  
GEV for response**

**Model  $\mu, \sigma, \xi$  with smooths of  
Year**

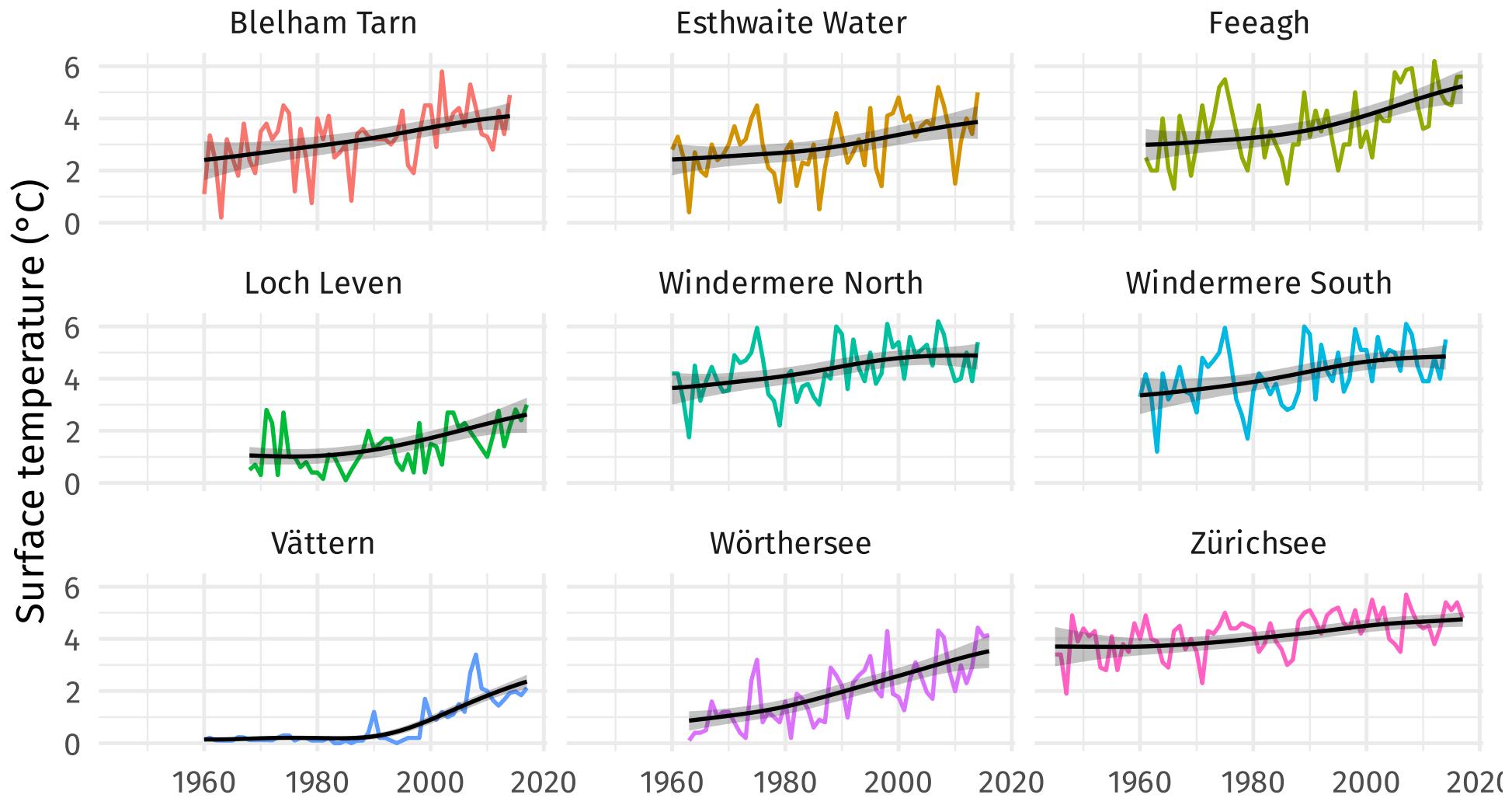
# Estimated smooths



# Observed vs fitted



# Estimated minimum temperature



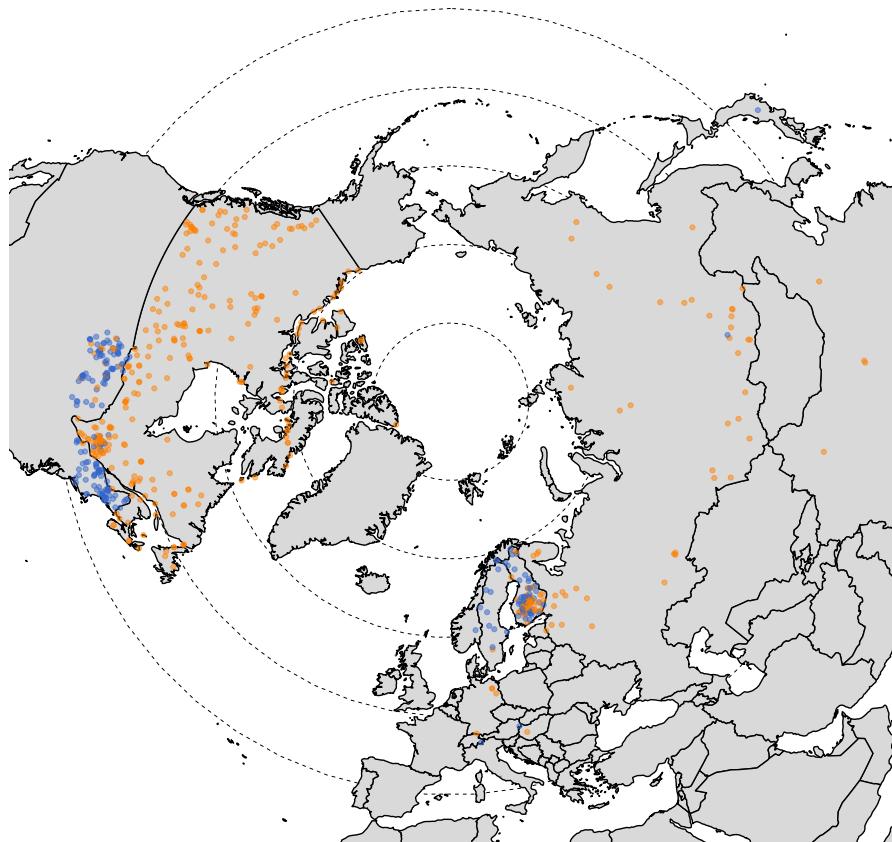
# Summary

- Lake **minimum** surface water temperatures have increased by on the order of 1–3 degrees over the last 60 years
- Evidence that the distribution of annual minima has changed in many lakes – implications for future extreme events which have long-term knock-on effects
- Distributional GAMs with the GEV distribution are an excellent way of modelling common trends in environmental extremes

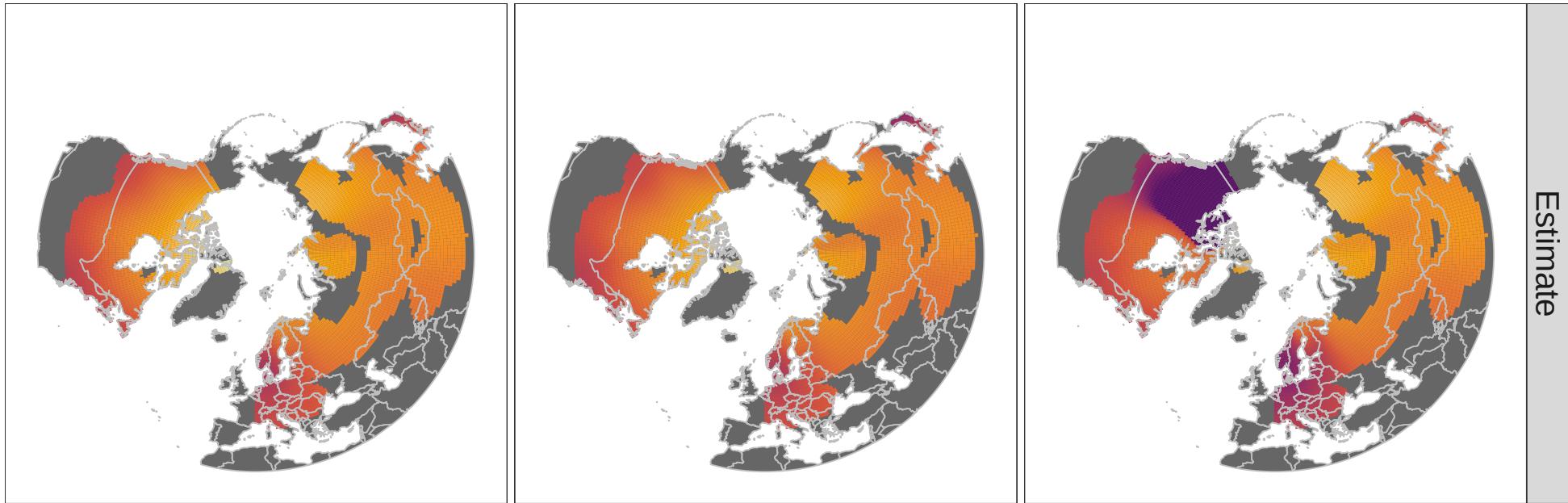
# Current research

1. The California Cooperative Oceanic Fisheries Investigations (CalCOFI) – Natalya Gallo (UCSD)
2. Changing Ice-Phenology in north hemisphere lakes – Stefano Mezzini (UofR)

Data after 1995 • FALSE • TRUE



# Ice Phenology

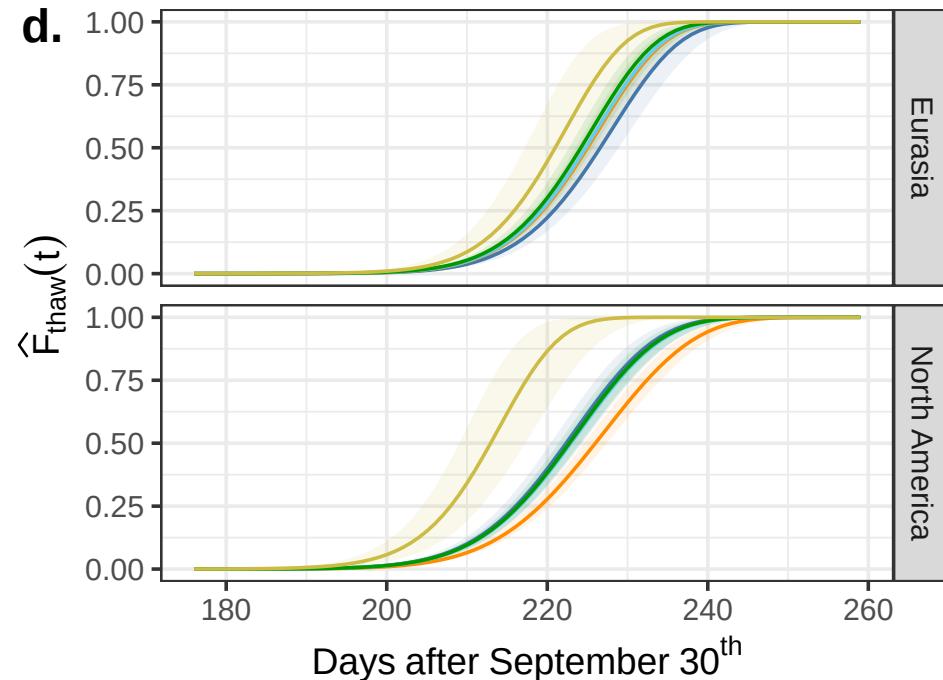
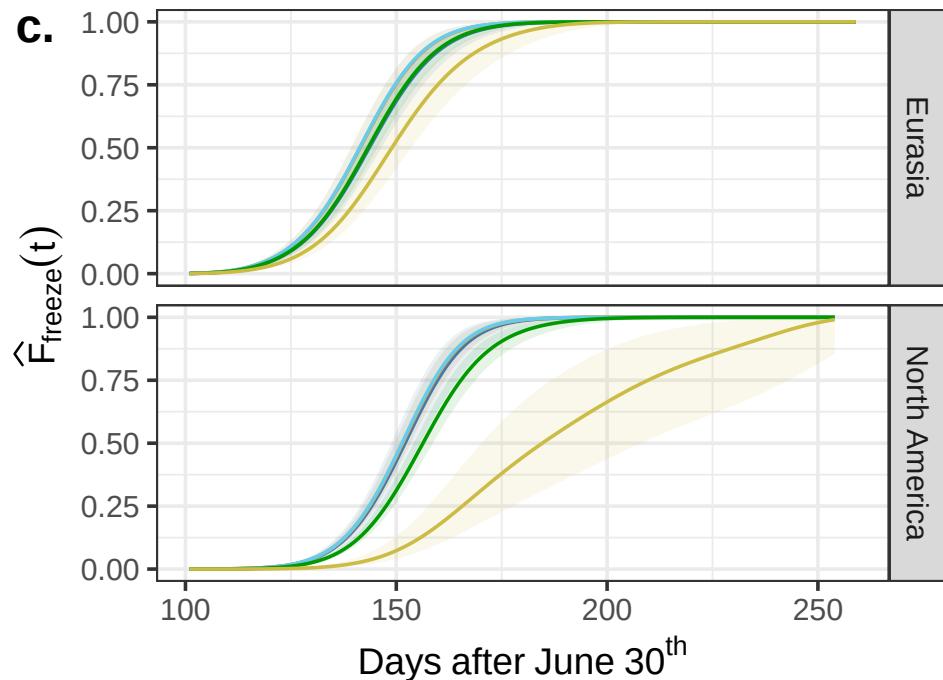


Mean freezing date  
(days after June 30<sup>th</sup>)

A horizontal color scale bar with a gradient from yellow to dark purple. Numerical labels are placed at regular intervals along the bar: 100, 150, 200, 250, and 300.

# Ice Phenology

Year 1950 1965 1980 1995 2010



# Acknowledgements

## Funding



**NSERC  
CRSNG**



FACULTY OF  
GRADUATE STUDIES  
& RESEARCH

## Data

- Peter Leavitt (URegina) for the Lake 227 Data
- Iestyn Woolway and colleagues for archiving the lake surface water data
- Lake ice data from Global Lake and River Ice Phenology Database (GLRIPD,  
<http://nsidc.org/data/G01377.html>)

## Slides

- HTML Slide deck [bit.ly/hifmb-talk](https://bit.ly/hifmb-talk) © Simpson (2020)

