Uncertainty Quantification

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Outline

- Introduction to UQ
- How to compute stuff
  - GP's
- A climate-macro application

Introduction to UQ

- Uncertainty quantification aims at studying the impact of aleatory (e.g. natural variability) or epistemic uncertainty onto computational models used in science and engineering (Saltelli et al. (2007), Sudret (2008))
- Does it make sense in economics? (Harenberg et al. (2019))
  - In Climate-Macro? (Miftakhova (2021))

Parametric model uncertainty

- Consider a generic model $\mathscr{M}(\cdot)$ which has N uncertain parameters $\theta \in \boldsymbol{\Theta} \subset \mathbb{R}^N$ as an input and model outputs $y \in \mathbb{R}^k$ (the QoI)
- Given a cdf over Θ, what is the distribution of y?

Uncertainty Quantification

- Given a distribution over uncertain parameter, what's the variance of the quantities of interest (QoI)
- Typical complaint: In many economic models this variance is so large that quantitative statements are meaningless

Uncertainty Quantification

- Which input parameters contribute the most to the variance?
  - Sobol indices and Shapley value
  - If large, need better data or change model

Functional ANOVA (Hooker (2004))

- Want to decompose (squ. integrable) $\hat{f} : \mathbb{R}^p \mapsto \mathbb{R}$ as

$$\hat{f}(x) = \sum_{S \subseteq \{1,\ldots,p\}} \hat{f}_S(x_S)$$

$$= C + \hat{f}_1(x_1) + \ldots + \hat{f}_p(x_p) + \hat{f}_{1,2}(x_1, x_2) + \hat{f}_{1,3}(x_1, x_3) + \ldots + \hat{f}_{1...p}(x)$$

Functional ANOVA (Hooker (2004))

- Want to decompose (squ. integrable) $\hat{f} : \mathbb{R}^p \mapsto \mathbb{R}$ as

$$\hat{f}(x) = \sum_{S \subseteq \{1,\ldots,p\}} \hat{f}_S(x_S)$$

- Define recursively

$$\hat{f}_S(x) = \int_{X_{-S}} \left(\hat{f}(x)\right) dX_{-S} - \int_{X_{-S}} \left(\sum_{V \subset S} \hat{f}_V(x)\right) dX_{-S}$$

Functional ANOVA (cont)

- Start with intercept:

$$\hat{f}_0(x) = \int_X \hat{f}(x) dX$$

- Univariate terms:

$$\hat{f}_i(x) = \int_{X_{-i}} \left(\hat{f}(x) - \hat{f}_0 \right) dX_{-S}$$

- Etc

ANOVA and Sobol

- Easy to see that for all non-empty S
$\int \hat{f}_S(x_S)dX_s = 0$ and that for all $S \neq V$
$\int \hat{f}_S(x_S)\hat{f}_V(x_v)dX = 0$

- Now let's take X to be a random variable and we get (with independence)
$\sigma^2(\hat{f}) = \sum_{S \subseteq \{1,\ldots,p\}} \sigma_S^2(\hat{f}_S)$

Sobol Index

- The first-order Sobol indices are:

$$S_i = \frac{\mathrm{Var}_{\theta_i}\left[\mathbb{E}_{\Theta\backslash\theta_i}\left[y \mid \theta_i\right]\right]}{\mathrm{Var}_{\Theta}\left[y\right]}$$

- Higher orders can be defined in the same way, but the number of these indices grows fast
    - Not exactly what we want...

Shapley Value

- A cooperative game in characteristic function form: Finite set of players N={1,...,n}. Characteristic function v defined on all subsets of N.
- Standard restrictions such as superadditivity
- Want to find the value of the game for each player

Shapley Value (cont)

- Shapley proposed 3 axioms: symmetry, carrier axiom and additivity axiom and showed that the value is uniquely determined by

$$\phi_i(v) = \sum_{S \subset N} \frac{(s-1)!(n-s)!}{n!}[v(S) - v(S-i)]$$

Shapley value and UQ (e.g. Owen(2014))

- What is the Shapely value of each input parameter?
- Do the axioms make sense in this context?
  - Not so clear for additivity, but Young (1985) replaces is with a marginality principle...

Marginality

- Define $v_i(S) = v(S + i) - V(S)$

- Marginality principle: For any 2 games, v,w $v_i = w_i \Rightarrow \phi_i(v) = \phi_i(w)$

How to compute?

- Need to solve model for a (possibly large) number of parameters
  - Using neural nets, one might be able to include them as states and solve the problem only once
- And/ or build efficient surrogate model
  - → Gaussian processes

Radial basis functions

- Given any (non-empty) subset of Euclidean space, A, a (symmetric positive definite) kernel is a function $K : A \times A \to \mathbb{R}$ with $K(x, y) = K(y, x)$ for all x, y and $A_{K,X} = (K(x_j, x_k))_{j,k=1,\ldots,N}$ being positive definite for any finite subset of distinct points in A.
- Example: $k(x, x') = \exp\left(-\frac{1}{2}\sum_{i=1}^{k}\left(x_i - x_i'\right)^2\right).$
- Easy to see that given N points there are coefficients so that $f(x) = \sum_{i=1}^{N} \alpha_i K(x_i, x)$ interpolates!

Gaussian processes

- Rasmussen and Williams (2005) is standard reference (see also Scheidegger and Bilionis (2019))
- A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution
- Completely specified by its mean function m(x) and covariance function k(x,x')

Gaussian processes

$$E(f(x)) = m(x), Cov(f(x), f(x')) = k(x, x') \Rightarrow f(x) \sim \mathcal{GP}(m(x), k(x, x'))$$

cs.toronto.edu

The Kernel Cookbook:

Advice on Covariance functions

by David Duvenaud

$$k_{\mathrm{SE}}(x, x') = \exp\left\{ -\frac{1}{2} \sum_{i=1}^{d} \frac{(x_i - x_i')^2}{\ell_i^2} \right\}$$

$$k_{\mathsf{mat}}(x, x') = \sigma^2 \left(1 + \sqrt{3} \sum_{i=1}^{l} \frac{\left(x_i - x_i'\right)^2}{\ell_i^2} \right) \exp\left(-\sqrt{3} \sum_{i=1}^{l} \frac{\left(x_i - x_i'\right)^2}{\ell_i^2} \right),$$

Gaussian processes

$$E(f(x)) = m(x), Cov(f(x), f(x')) = k(x, x') \Rightarrow f(x) \sim \mathcal{GP}(m(x), k(x, x'))$$

Observations (x^i, y^i), $y^i = f(x^i) + \epsilon^i$

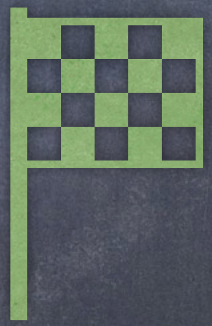
normal with std s

$$\begin{pmatrix} y \\ f(x) \end{pmatrix} \sim \mathcal{N}\left(0, \begin{pmatrix} K(X,X) + s^2 I & K(X,x) \\ K(x,X) & k(x,x) \end{pmatrix}\right)$$

Gaussian processes

$$f(x)|X, y, s \sim \mathcal{N}\left(\tilde{m}(x), \tilde{\sigma}^2(x)\right)$$

$$\tilde{m}(x) = K(x, X)\left(K(X, X) + s^2 I\right)^{-1} y$$



That is our approximation

Computing Shapely Value and Sobol Indices

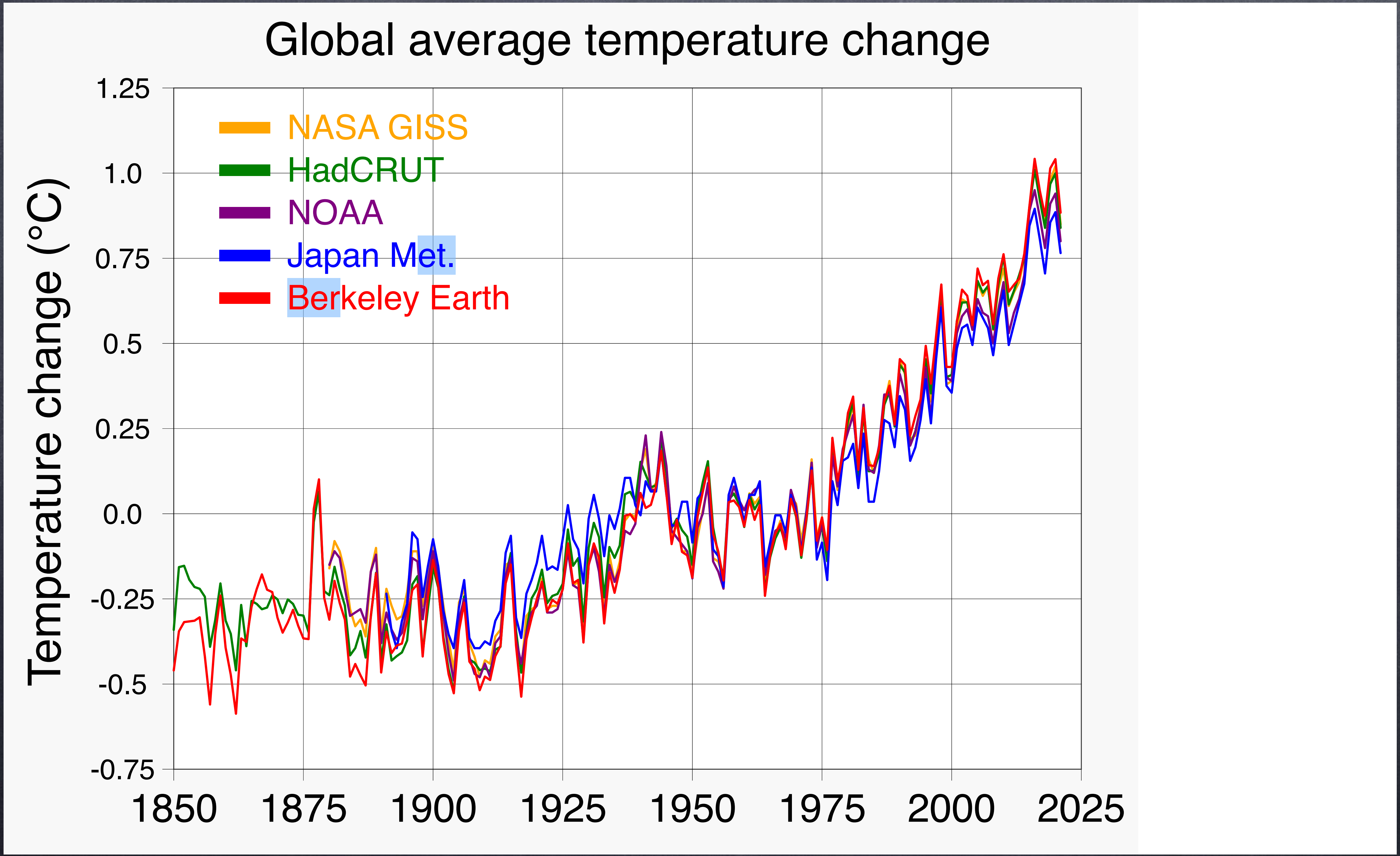
- We generate M model input-output pairs to obtain the training dataset $\mathscr{D} = \{\theta_i, y_i\}_{i=0}^{M}$
- We fit the GP model on the training data and write it as $\mathscr{M}_{\mathrm{GP}|\Theta,Y}$
- Leave-out error to evaluate accuracy

LOO

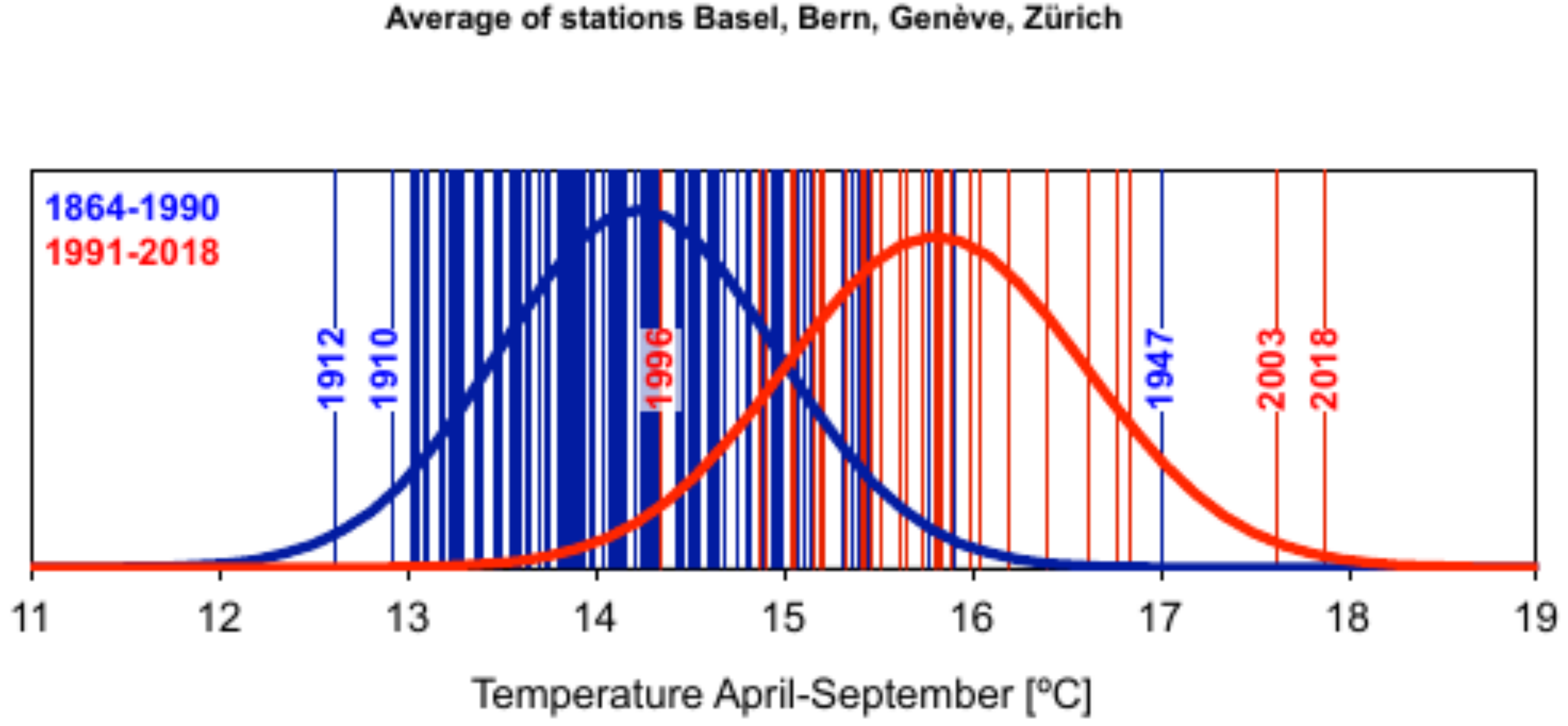
- To measure the LOO error, we first construct GP surrogate models $\mathscr{M}_{\mathrm{GP}|\theta_{-i},y_{-i}}$
- Define $\Delta_i \equiv \mathscr{M}(\theta_i) - \mathscr{M}_{\mathrm{GP}|\theta_{-i},y_{-i}}(x_i)$
- Define the LOO as $\epsilon_{\mathrm{LOO}}^{\mathrm{GP}} \equiv \dfrac{1}{M}\displaystyle\sum_{i=1}^{M} \Delta_i^2$

Numerical Integration

It's warming and it's us



Really!



Schär, ETH Zürich (updated from Schär et al. 2004, *Nature*, **427**, 332-336); Station observations from MeteoSwiss

The Nordhaus program

- Postulate planners problem: Single infinitely lived agent maximises utility from consumption. Firm produces and emits CO2.
- Reducing emission is costly but reduces future damages from warming
- How much money should we spend on reducing emissions?

Some uncertainties

- Future emissions
- Climate (TCR, ECS, Tipping points, extreme weather)
- Damages

In a model with forward looking, utility maximizing agents !!!!

2 kinds of uncertainty

- Model uncertainty
- Exogenous shocks

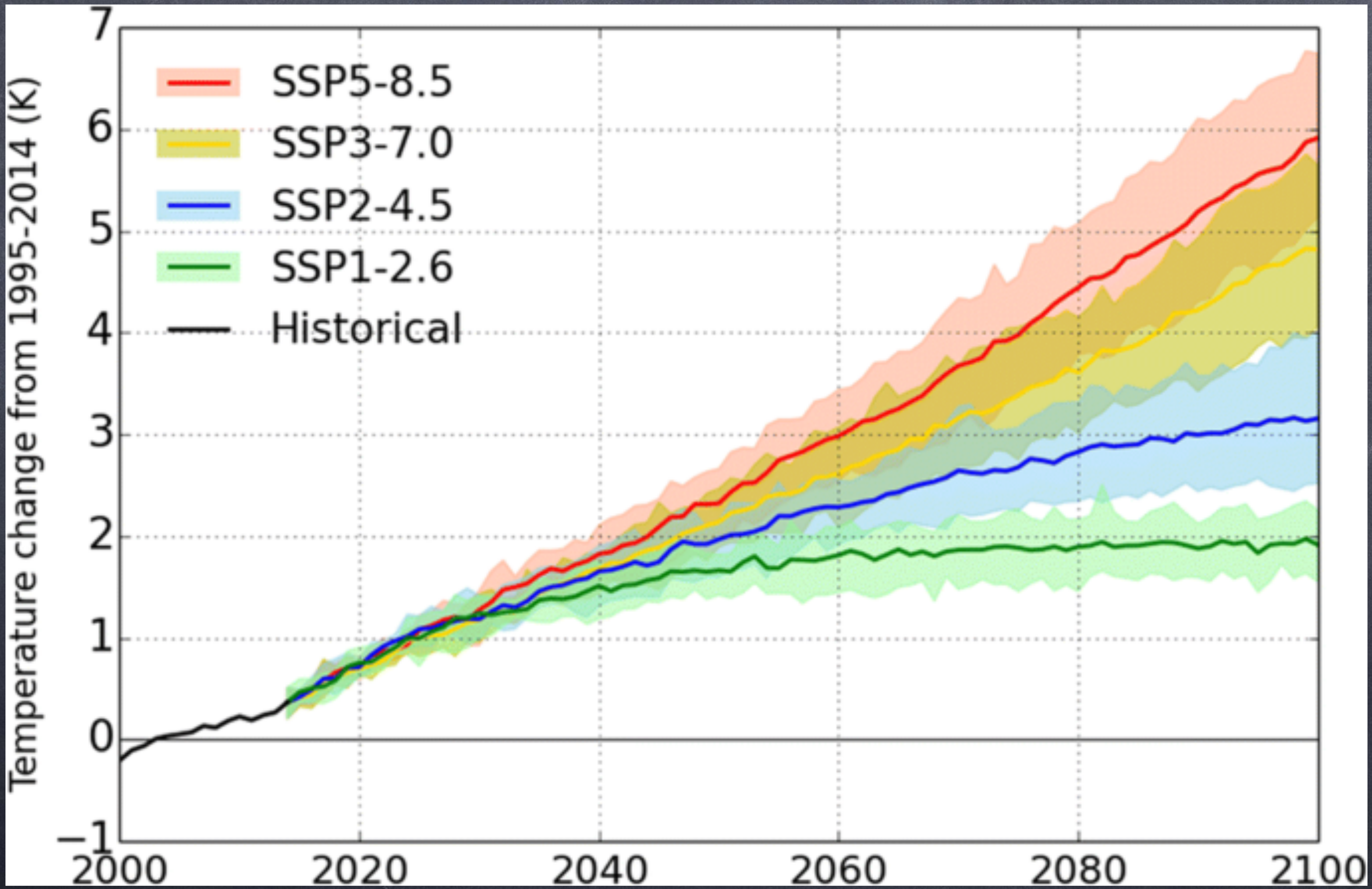
Climate models

- Scientists use AOGCM (atmosphere ocean global climate models) to assess the effect of higher CO2 concentration on temperature
- ESM (earth system models) are used to figure out how CO2 emissions leads to higher CO2 concentration
- simple climate models (or climate emulators) are a way to describe the data coming out of these. Economists need simple CEs

In CMIP we trust

- Research groups around the world submit simulations for predefined problems —> Coupled Model Intercomparison Project
- Calibrate CE to match the CMIP outputs

Climate Uncertainty



Climate Emulator

- 3-reservoir carbon cycle

$$\begin{pmatrix} J_t^A \\ J_t^U \\ J_t^L \end{pmatrix} = \Phi^J \begin{pmatrix} J_{t-1}^A \\ J_{t-1}^U \\ J_{t-1}^L \end{pmatrix} + \begin{pmatrix} \varrho^O O_t + \varrho^G G_t + \varrho^{\mathscr{C}} \mathscr{C}_t + E_t^{Land} \\ 0 \\ 0 \end{pmatrix}.$$

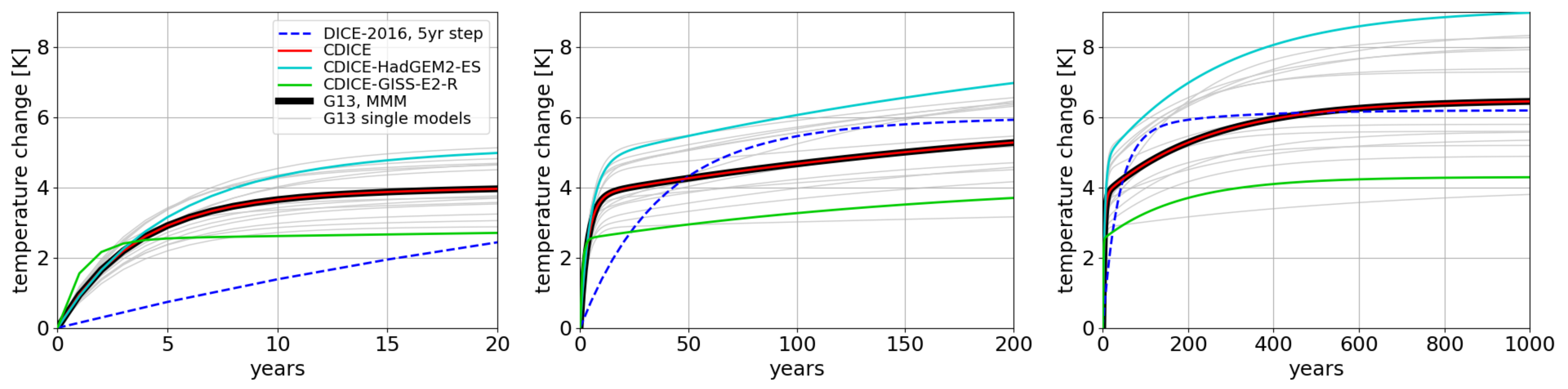
- Forcing: $F_t = \eta_1 \dfrac{\log \frac{J_t^A}{J^0}}{\log(2)} + F_t^{EX}$

- 2 layer Energy Balance Model for Temperature:

$$\begin{pmatrix} T_t^A \\ T_t^L \end{pmatrix} = \Phi^T \begin{pmatrix} T_{t-1}^A \\ T_{t-1}^L \end{pmatrix} + \begin{pmatrix} \eta_2 F_t \\ 0 \end{pmatrix}$$

Calibrating to CMIPs,

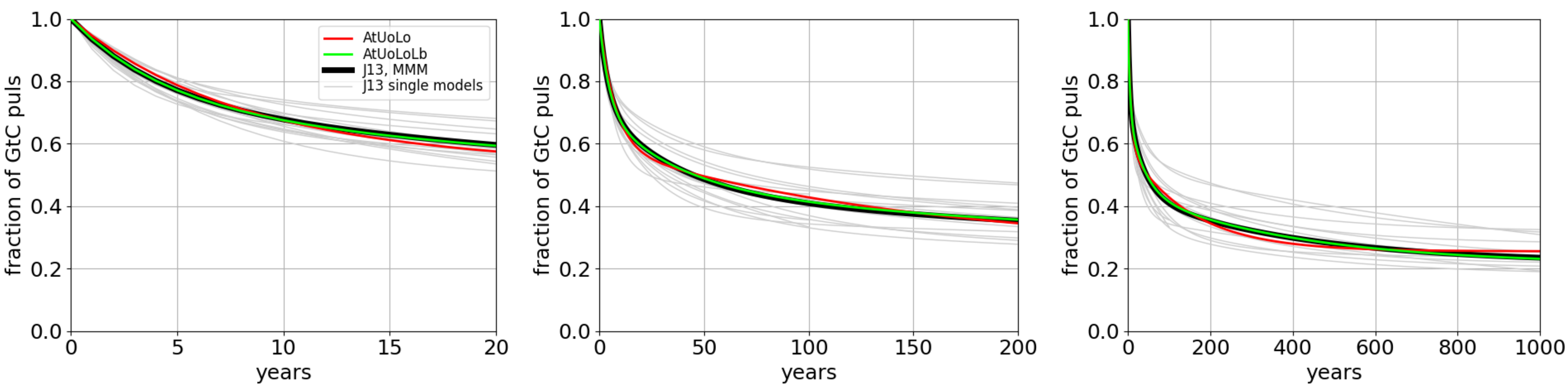
Folini et al (2022), Geoffrey et al (2013)



Temperature response to instantaneous quadrupling of atmospheric CO2 with respect to pre-industrial values on time scales of 20 years (left), 200 years (middle), and 1000 years (right). Parameters in CDICE (red solid) can be chosen such as to exactly reproduce the calibration targets

Carbon cycle

Folini et al (2022) Joos et al (2013)



Fraction of an instantaneous 100 GtC pulse remaining in the atmosphere (y-axis) as a function of time (x-axis, three different time scales from left to right).

Temperature

$$T_{t+1}^{\mathrm{AT}} = T_t^{\mathrm{AT}} + \Delta_t \cdot c_1 \left(F_t - \lambda T_t^{\mathrm{AT}} - c_3 \left(T_t^{\mathrm{AT}} - T_t^{\mathrm{OC}} \right) \right), \quad \lambda = F_{2XCO2}/ECS$$

	c_1	c_3	c_4	ECS
HadG	0.154	0.55	0.00671	4.55
MMM	0.137	0.73	0.00689	3.25
GISS	0.213	1.16	0.00921	2.15

Dynamic program

$$V\left(X_t\right)^{1-1/\psi} = \max_{C_t, K_{t+1}, \mu_t} \left\{ \left(\frac{C_t}{L_t}\right)^{1-1/\psi} L_t + e^{-\rho} \mathbb{E}_t \left[V\left(X_{t+1}\right)^{1-\gamma} \right]^{\frac{1-1/\psi}{1-\gamma}} \right\}$$

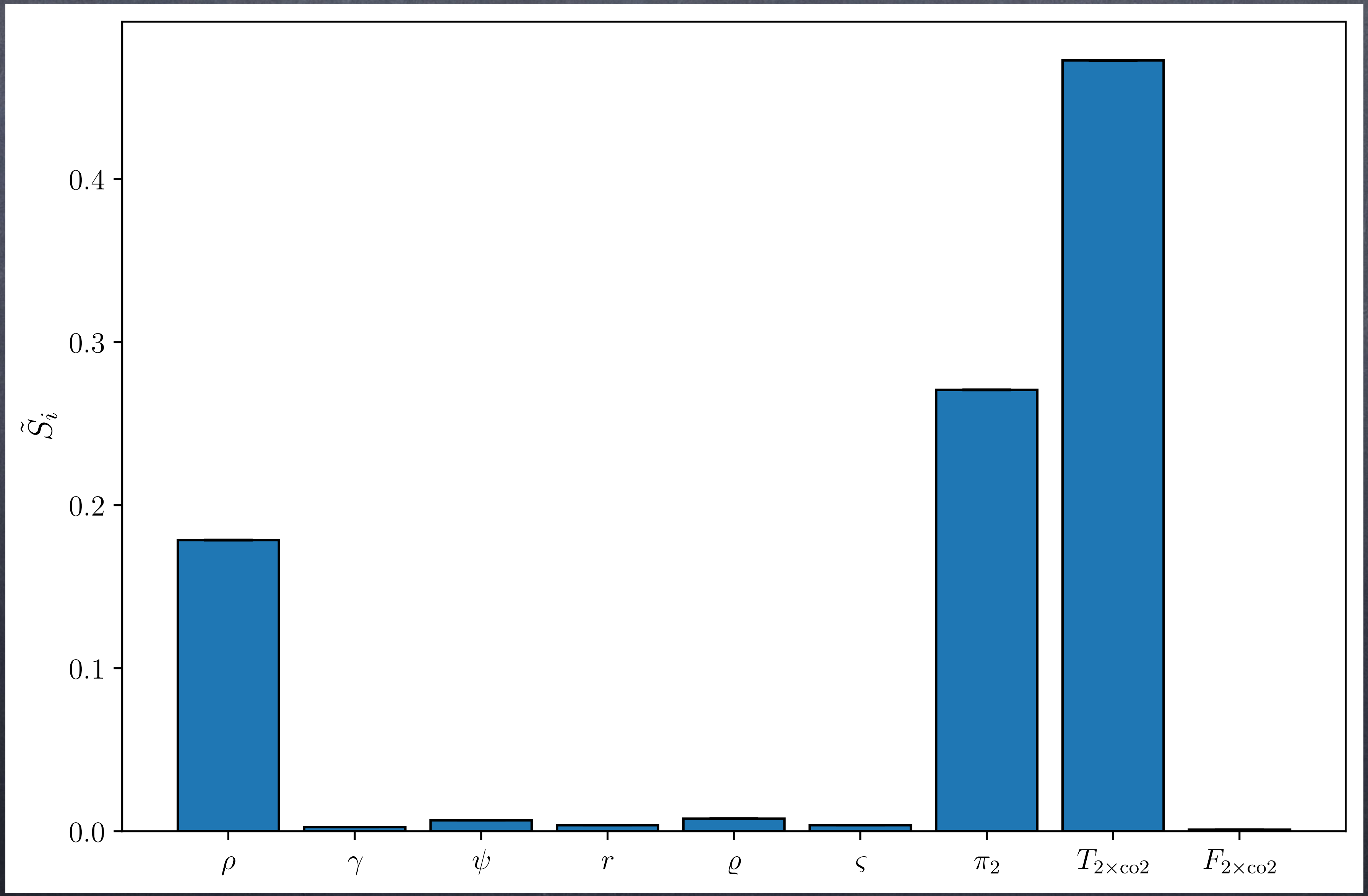
$$\Big(1 - \Theta\left(\mu_t\right)\Big) \Omega_t \left(T_{\mathrm{AT},t}\right) K_t^{\alpha} \left(A_t L_t\right)^{1-\alpha} - C_t - I_t = 0, \;\; (1-\delta) K_t + I_t - K_{t+1} = 0$$

$$\Omega\left(T_{\mathrm{AT},t}\right) = 1 - \pi_2 T_{\mathrm{AT},t}^2$$

+Climate

Sobol 1

Coefficient of variation 0.48



Simple uncertainty

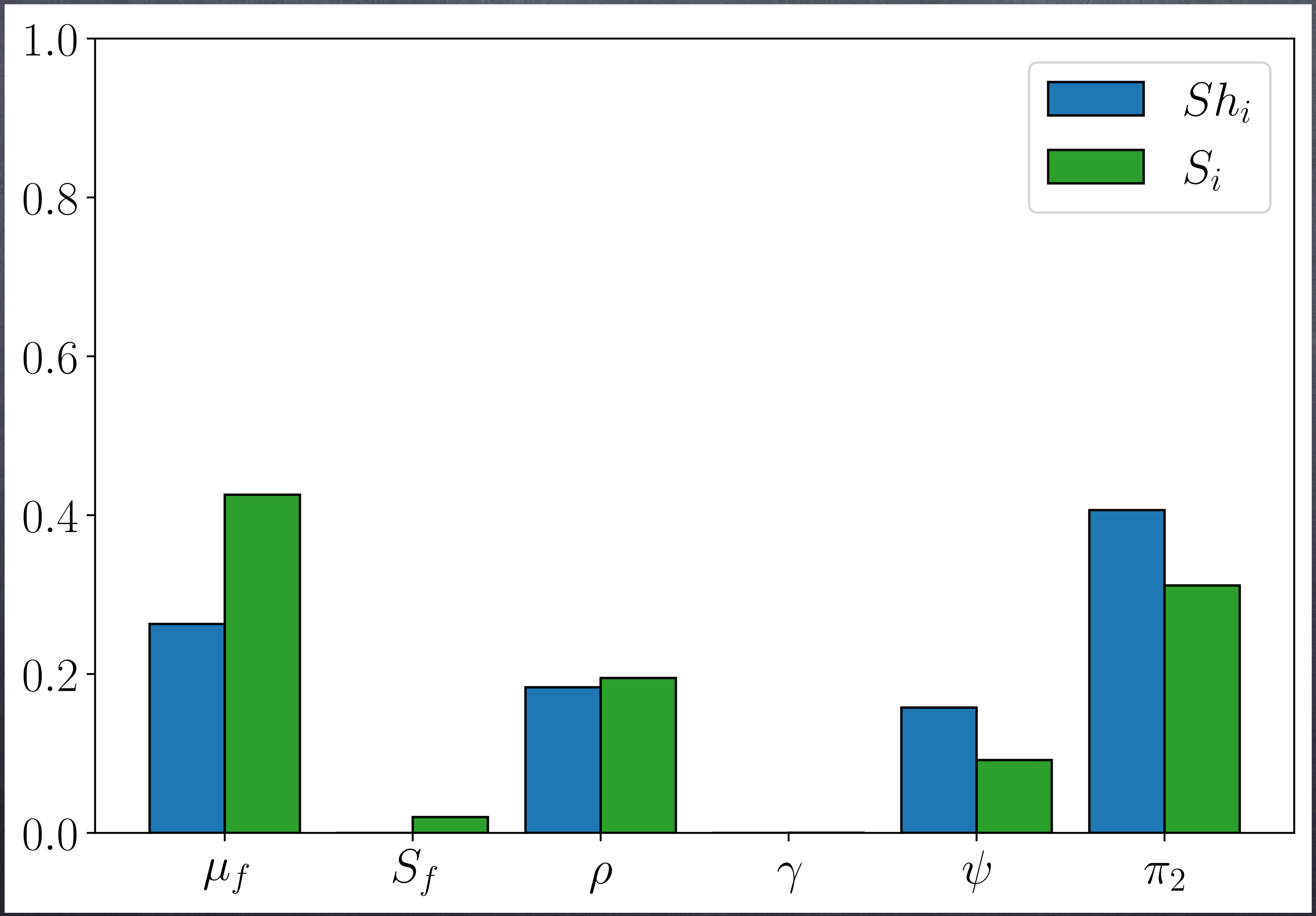
- Follow Roe and Baker (2007) to make ECS stochastic.
- $\text{ECS} = \frac{\lambda_0}{1-f} F_{2\text{XCO2}} \;\; f \sim \mathcal{N}\left(\bar{f}, \sigma_f^2\right)$
- This obviously makes no sense, see Ziliapin and Ghil (2006) but also Roe and Baker (2011) and Ziliapin and Ghil (2011)
- Truncate! Where? Here 0.85 (-> ECS 8)

Learning

(Kelly and Tan (2015), Hwang et al. (2017))

- $T_{t+1}^{\mathrm{AT}} = T_t^{\mathrm{AT}} + \Delta_t \cdot c_1 \left(F_t - \lambda_0 (1-f) T_t^{\mathrm{AT}} - c_3 \left(T_t^{\mathrm{AT}} - T_t^{\mathrm{OC}} \right) \right) + \epsilon_{t+1}$
- $$F_t = \eta_1 \frac{\log \frac{J_t^A}{J^0}}{\log(2)} + F_t^{EX0} + \eta_2 \xi_t$$
- Assume that the temperature shock is normal, an agent has truncated normal prior on f and uses Bayesian updating.
- Explicit simple formulas

UQ 2



Can figure out beliefs?