New climatology modeling methodologies

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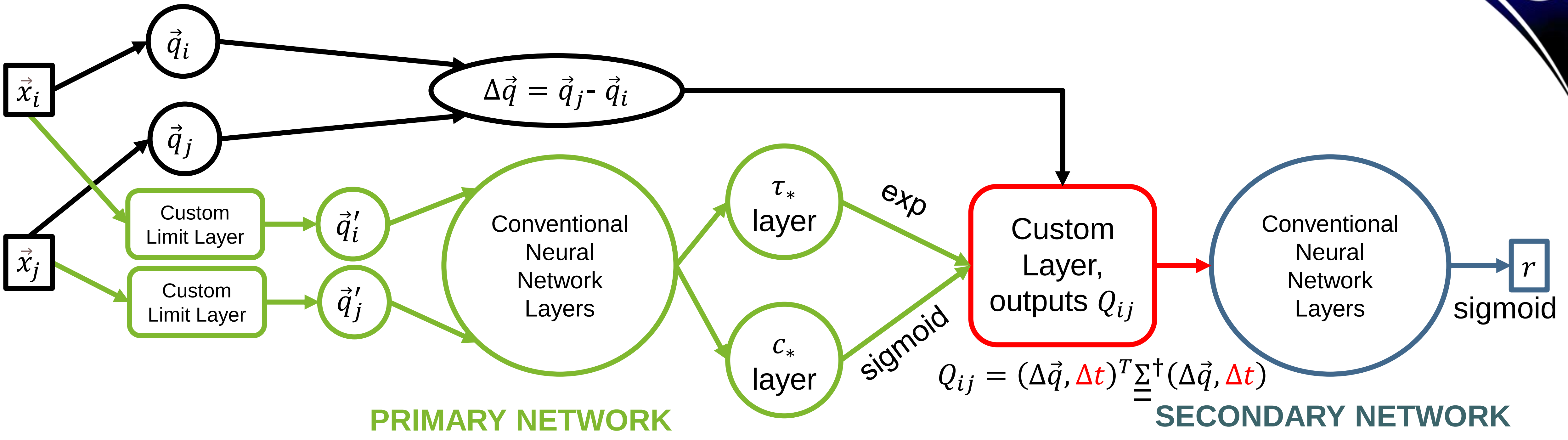
Analytical Covariance Matrices

Background

- Climatology models that go beyond a mean environment require spatial and spatiotemporal covariance to estimate confidence levels
- The model domains typically have 3 or 4 “spatial” dimensions, e.g., E, K, Φ
- For a 3-d model, the spatiotemporal covariance is a 7-dimensional function:
  - $r(x_1, x_2, x_3, x_1', x_2', x_3', \Delta t) = \mathrm{cov}\left(j(x_1, x_2, x_3, t), j(x_1', x_2', x_3', t + \Delta t)\right)$
  - j is flux or log flux or a Gaussian replacement of flux
  - This function has several constraints, for example, when $\Delta t = 0$ and $\vec{x} = \vec{x}'$, then $r =1$
- ONERA has a simplified solution [Brunet+2021]:
  - Obtain spatial correlations from a simulation (Salammbo) and data set (Van Allen Probes)
  - Obtain spatiotemporal correlations with a temporal decorrelation function fitted to data
  - $r(x_1, x_2, x_3, x_1', x_2', x_3', \Delta t) = \mathrm{cov}\left(j(x_1, x_2, x_3, t), j(x_1', x_2', x_3', t)\right) \exp\left(-\frac{\Delta t^2}{2\tau(x_1,x_2,x_3)\tau\left(x_1',x_2',x_3'\right)}\right)$
  - Does not handle asymmetric temporal correlations
  - Cannot interpolate or extrapolate spatially if the simulation or data set do not cover the entire domain of the climatology model
- We expand on prior works in Gaussian Processes [Paciorek+Schervish, 2004; Rasmussen+Williams, 2006] to develop a flexible non-stationary covariance function in the form of a neural network
- We train the neural network with data from a numerical simulations, electrons so far:
  - VERB [Saikin+2021] that uses a V, K, L coordinate system (already in use)
  - BAS-RBM [Glauert+2018] uses E, K, L* coordinate system (not yet in use)

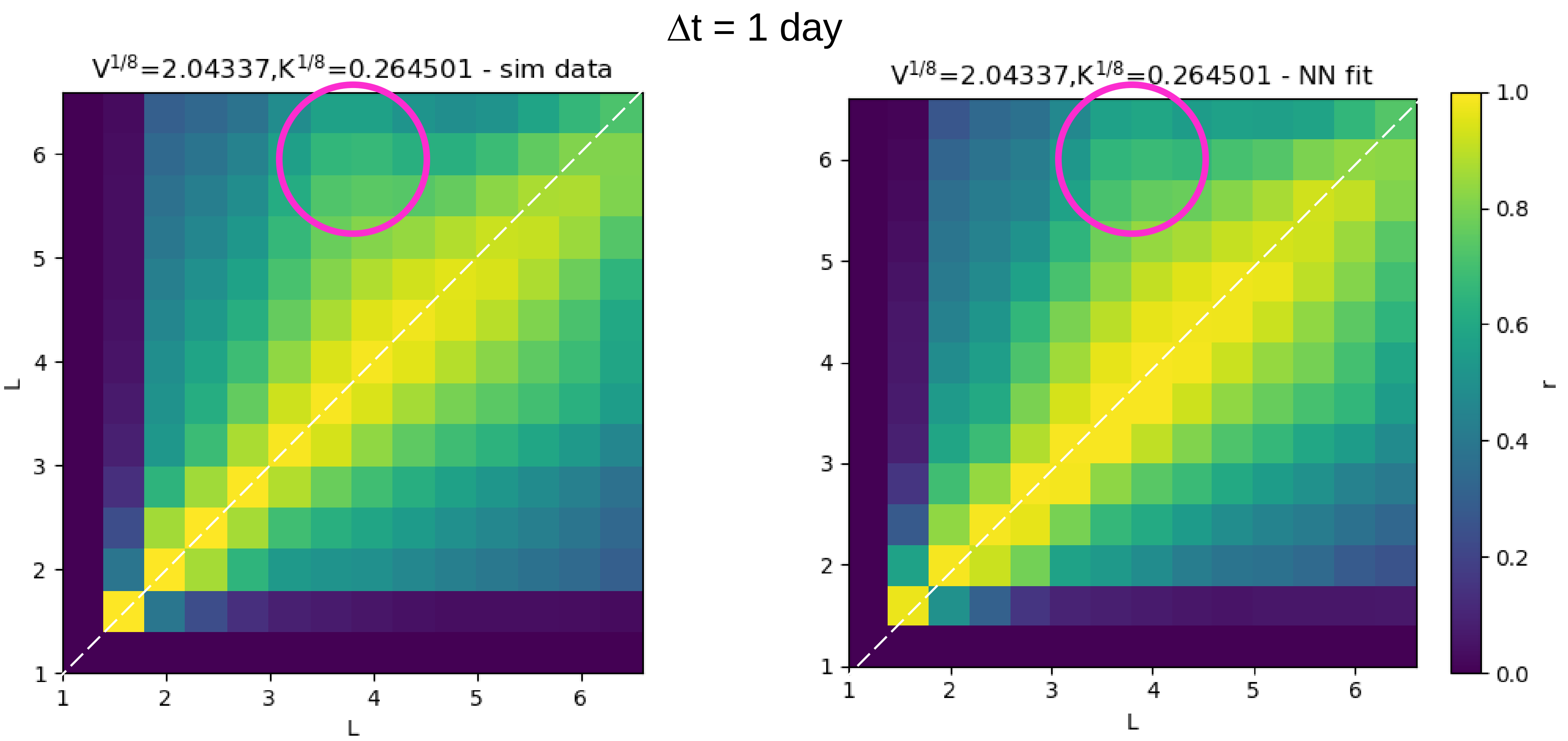
Neural network model of spatio-temporal covariance



- We extend the space to a fourth dimension (Δt), which allows for $\mathrm{r}(\vec{x}_i, \vec{x}_i; \Delta t) < 1$
- We can employ an input swap requirement to ensure symmetry $\mathrm{r}\left(\vec{x}_i, \vec{x}_j; \Delta t\right) = \mathrm{r}\left(\vec{x}_j, \vec{x}_i; -\Delta t\right)$
- We train a separate network at each Δt. In practice the network only knows that $\Delta t > 0$, and actually uses Δt=1 in all cases for numerical stability. The real value of Δt is only used to build training data and to label the network

$$\underline{\underline{\Sigma}} = \begin{bmatrix} \tau_1^2 & c_{12}\tau_1\tau_2 & c_{13}\tau_1\tau_3 & c_{1t}\tau_1\tau_t \\ c_{12}\tau_1\tau_2 & \tau_2^2 & c_{23}\tau_2\tau_3 & c_{2t}\tau_2\tau_t \\ c_{13}\tau_1\tau_3 & c_{23}\tau_2\tau_3 & \tau_3^2 & c_{3t}\tau_3\tau_t \\ c_{1t}\tau_1\tau_t & c_{2t}\tau_2\tau_t & c_{3t}\tau_3\tau_t & \tau_t^2 \end{bmatrix}$$

Example NN Spatio-Temporal Covariance Fit (1 day time lag)

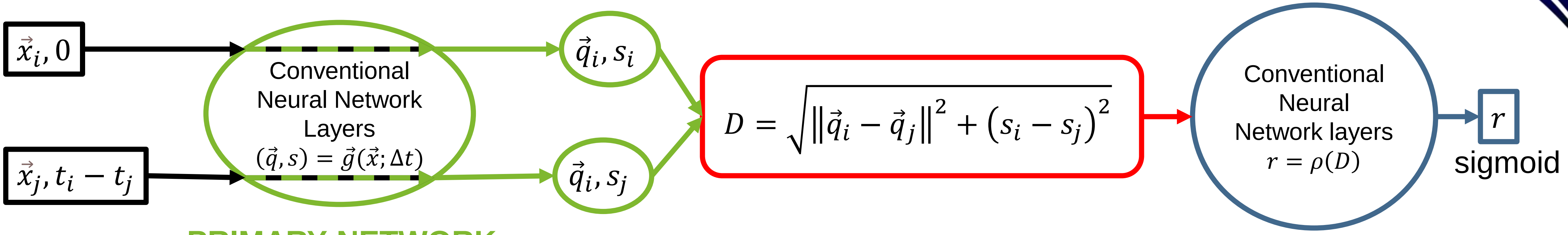


NN covers all V, K, L in sim. Only one slice shown here.
Notice slight asymmetry across diagonal, circled O

A new idea inspired by Reimann spaces

- Build a space-time coordinate transform to a system where decorrelation is isotropic (a "flat" space):
  - $(\vec{q}, s) = \vec{g}(\vec{x}; \Delta t)$
  - $r(\vec{q}_i, \vec{q}_j, t_i - t_j) = \rho\left(\sqrt{\left\|\vec{q}_i - \vec{q}_j\right\|^2 + \left(s_i - s_j\right)^2}\right)$
- Constraints:
  - $\frac{\partial g_i}{\partial x_i} > 0$ (monotonic)
  - $\frac{\partial g_i}{\partial x_j} = \frac{\partial g_j}{\partial x_i}$ (symmetric)
  - $\left|\frac{\partial \vec{g}}{\partial \vec{x}}\right| > 0$(non-singular matrix determinant)
  - $\rho(0) = 1$ (consistent)
  - $\vec{\nabla}\rho \cdot \vec{\nabla}\left(\sqrt{\left\|\vec{q}_i - \vec{q}_j\right\|^2 + \left(s_i - s_j\right)^2}\right) < 0$ (decorrelation with distance)
- Implementing constraints is fairly easy in modern NN codes (e.g., PyTorch): it's just another term in the penalty function
- Constraints can/should be applied over entire valid range of $\vec{x}, \Delta t$, not just where there's data
- This approach avoids a lot of the structural complexity of the prior approach, but it should be able to capture the same structural details – a spatial transform of this type is implicit in the 7-D covariance function

Reimann-inspired NN model of spatio-temporal covariance



PRIMARY NETWORK (Called twice)

$$\frac{\partial g_i}{\partial x_i} > 0 \qquad \frac{\partial g_i}{\partial x_j} = \frac{\partial g_j}{\partial x_i} \qquad \left|\frac{\partial \vec{g}}{\partial \vec{x}}\right| > 0$$

SECONDARY NETWORK

$$\rho(0) = 1 \qquad \frac{d\rho}{dD} < 0$$

- This neural network can be trained on the entire data set of correlations
  - Training tuples: $(\vec{x}_i, t_i, \vec{x}_j, t_j) \rightarrow r$
  - Observed correlations
  - Model correlations
  - Constraints
- Constraints should be applied at points within the domain randomized at every training step
- Weighting strategy among observed correlations, model correlations, and constraints will likely require some hand tuning

What we learned about using simulation data

- Sims often include a boundary region to separate the main physics domain from highly uncertain boundary conditions. Correlations computed in this boundary region are not valid and must be excluded from training data.
- The VERB sim appears to have certain grid points with anomalously low/no variation. Correlations involving these points are not valid and must be excluded from training data.
- The VERB sim appears to require a few years to “warm up”, especially at low L. Correlations should be computed only after this warm-up period.

New Marginal Distributions for Climatology Models

Acknowledgement: Constantinos Papadimitriou of SPARC contributed substantially to the investigation of new approaches to marginal distributions.

Introduction

- Marginal distributions describe the variability of particle flux at a specific point in the climatology model's grid
- Current climatology models take two different approaches to marginal distributions:
  - Tables of fluxes at prescribed percentiles
  - Parameters of analytical distributions (e.g., Weibull, Log-Normal which have 2 parameters)
- Tables are more precise, but it is complex to represent the uncertainty on them: $O(N^2)$ problem for table of N percentiles
- Parameters are easier to work with, but are less precise and have discontinuities if different functional forms are used for the same species (e.g., plasma electrons and radiation belt electrons)
- With Constantinos Papadimitriou at SPARC, we have developed a hybrid approach that combines tables for describing the marginal distribution with a 2-parameter approach to uncertainty

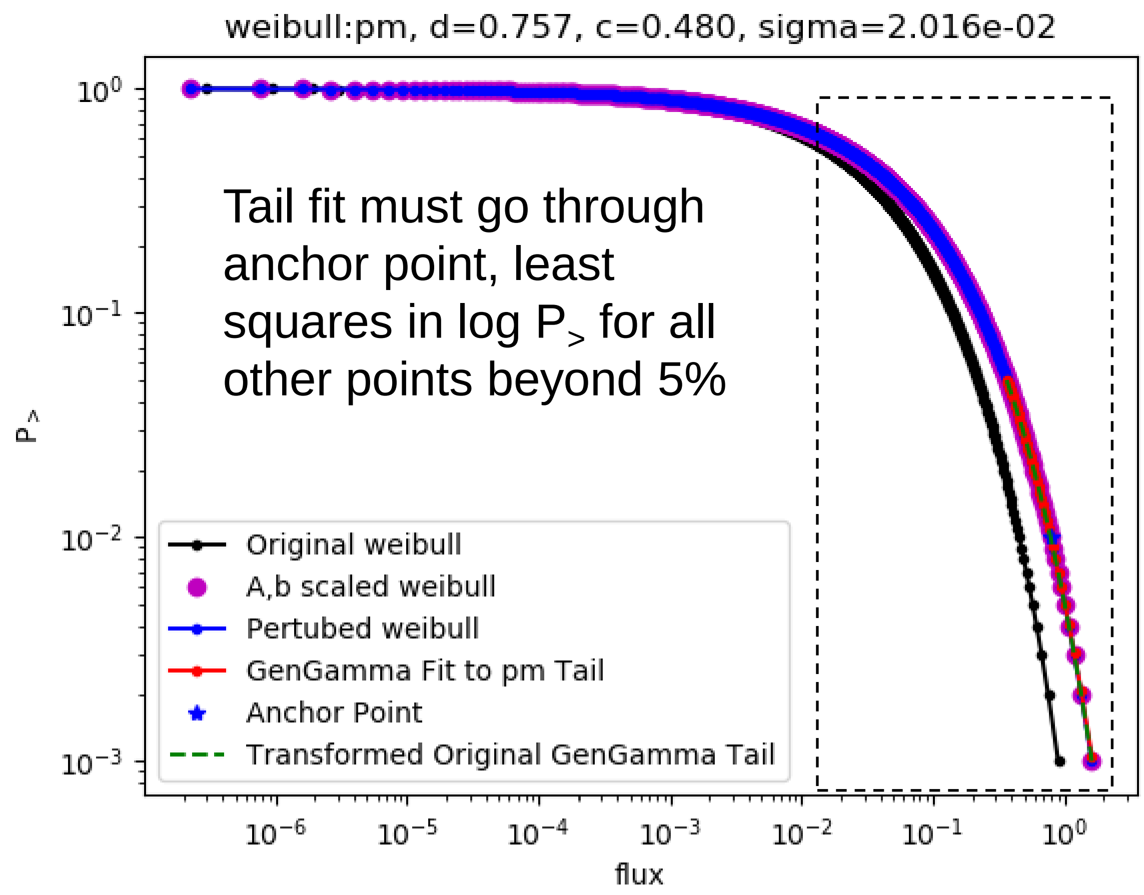
- Briefly: the marginal distribution is given as a table with a generalized gamma distribution* as its tail, while the uncertainty is tracked only for the 50^{th} and 95^{th} percentile. To perturb the entire distribution, first perturb the 50^{th} and 95^{th} percentiles, then interpolate/extrapolate those changes (in a power-law sense) to other percentiles

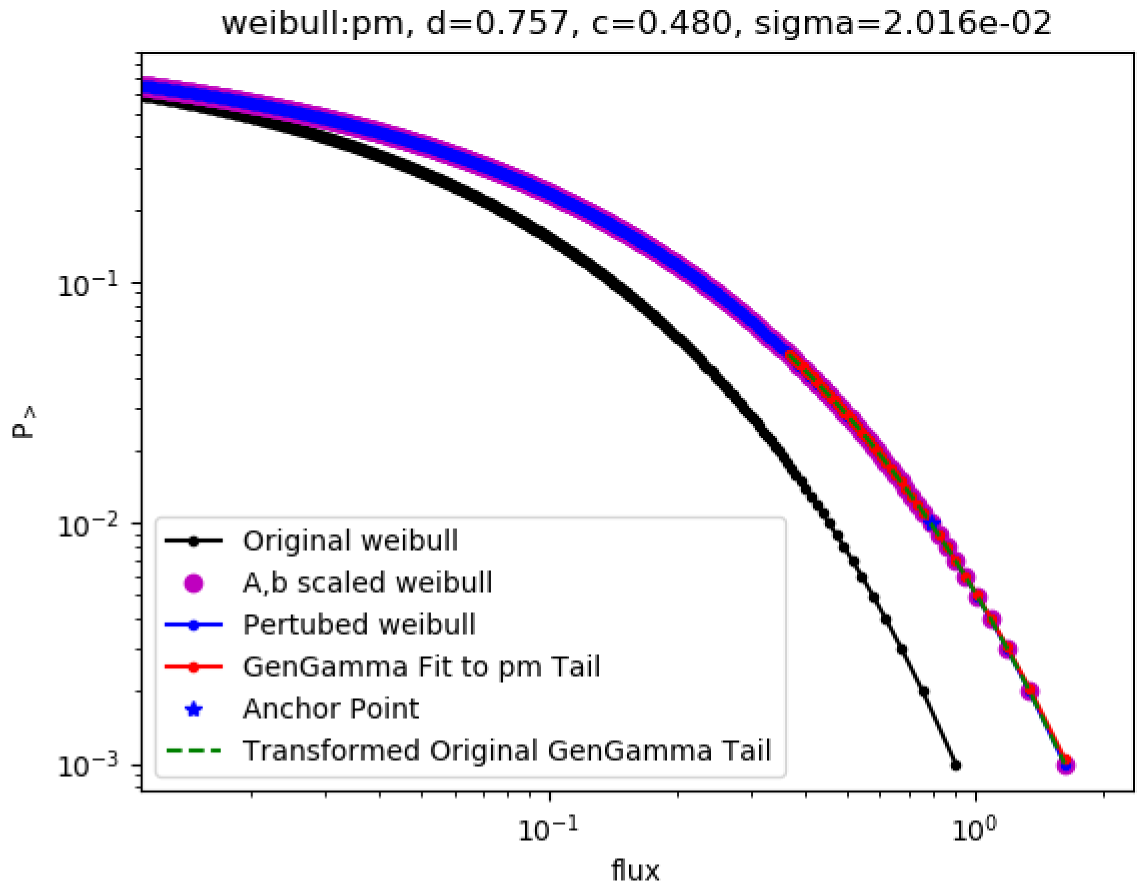
- *generalized gamma is a gamma distribution with a power-law transform applied to the variate

Math

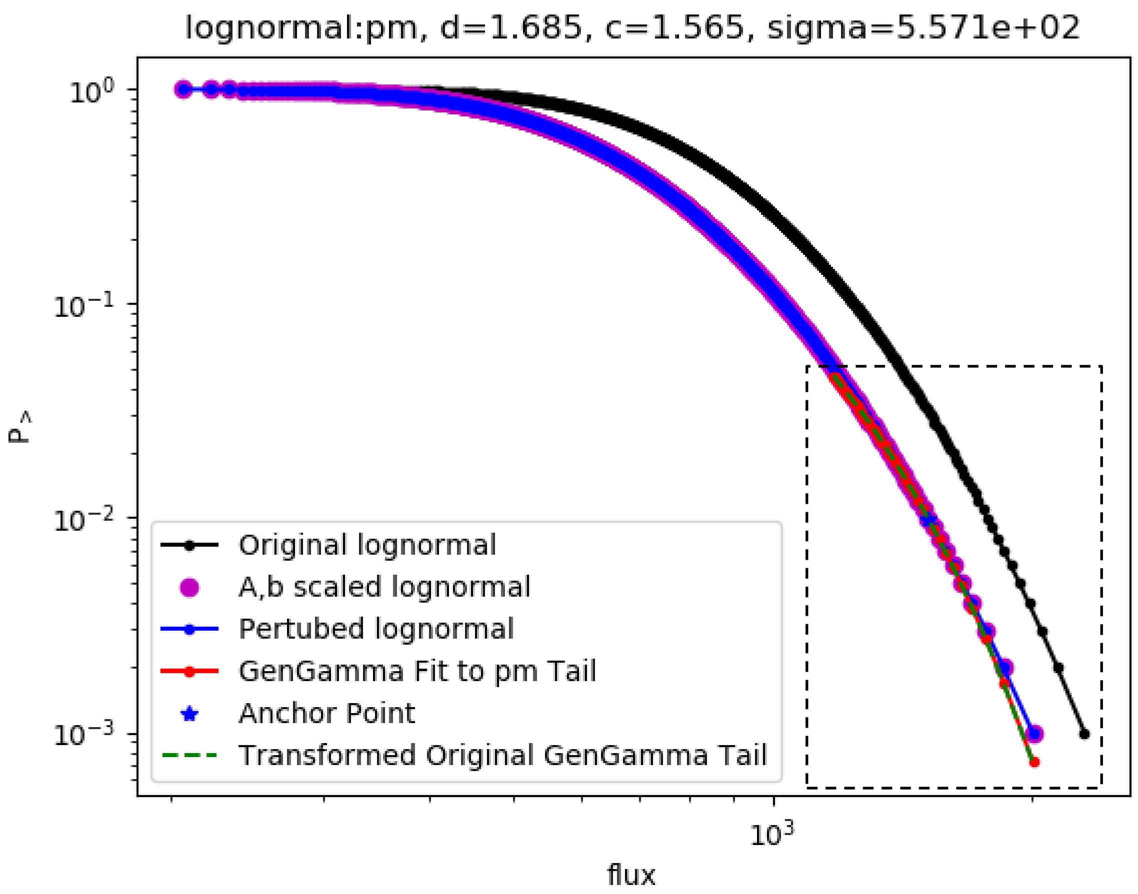
- At each grid point, we have a table of percentiles: $\vec{m} \in \{F(m_i) = p_i\}$
  - m_i is the flux at percentile p_i
  - m_{50} denotes the median, and m_{95} denotes the 95th percentile
- Error is represented on transformed variables:
  - $\theta_1 = \ln m_{50}, \theta_2 = \ln(m_{95} - m_{50})$
  - Global error matrix $\underline{\underline{S}}_\Theta$ tracks correlated errors at all grid points for θ_1 and θ_2
  - Perturb all θ using: $\vec{\Theta}' = \vec{\Theta} + \underline{\underline{S}}_\Theta \vec{\varepsilon}$, then obtain m'_{50} and m'_{95} at each grid point
- Assume a power-law perturbation function: $m'_i = A{m_i}^b$
  - $b = \ln \frac{m'_{50}}{m'_{95}} / \ln \frac{m_{50}}{m_{95}}$,$A = \frac{m'_{50}}{{m_{50}}^b}$
  - Apply this transform to all percentiles: $\vec{m}' \in \left\{F'(m'_i) = F'\left(A{m_i}^b\right) = p_i\right\}$
- Tail:
  - Original generalized gamma is: $F(x) = \gamma\left(\frac{d}{c}, \left(\frac{x}{\sigma}\right)^c\right) / \Gamma\left(\frac{d}{c}\right)$
  - Weibull when $\frac{d}{c} = 1$, log-normal as $\frac{d}{c} \to \infty$
  - Perturbed is $F'\left(x' = Ax^b\right) = \gamma\left(\frac{d\prime}{c\prime}, \left(\frac{x\prime}{\sigma\prime}\right)^{c\prime}\right) / \Gamma\left(\frac{d\prime}{c\prime}\right)$, $\sigma' = A\sigma^b, c' = c/b,\ d' = d/b,\ \frac{d'}{c'} = \frac{d}{c}$

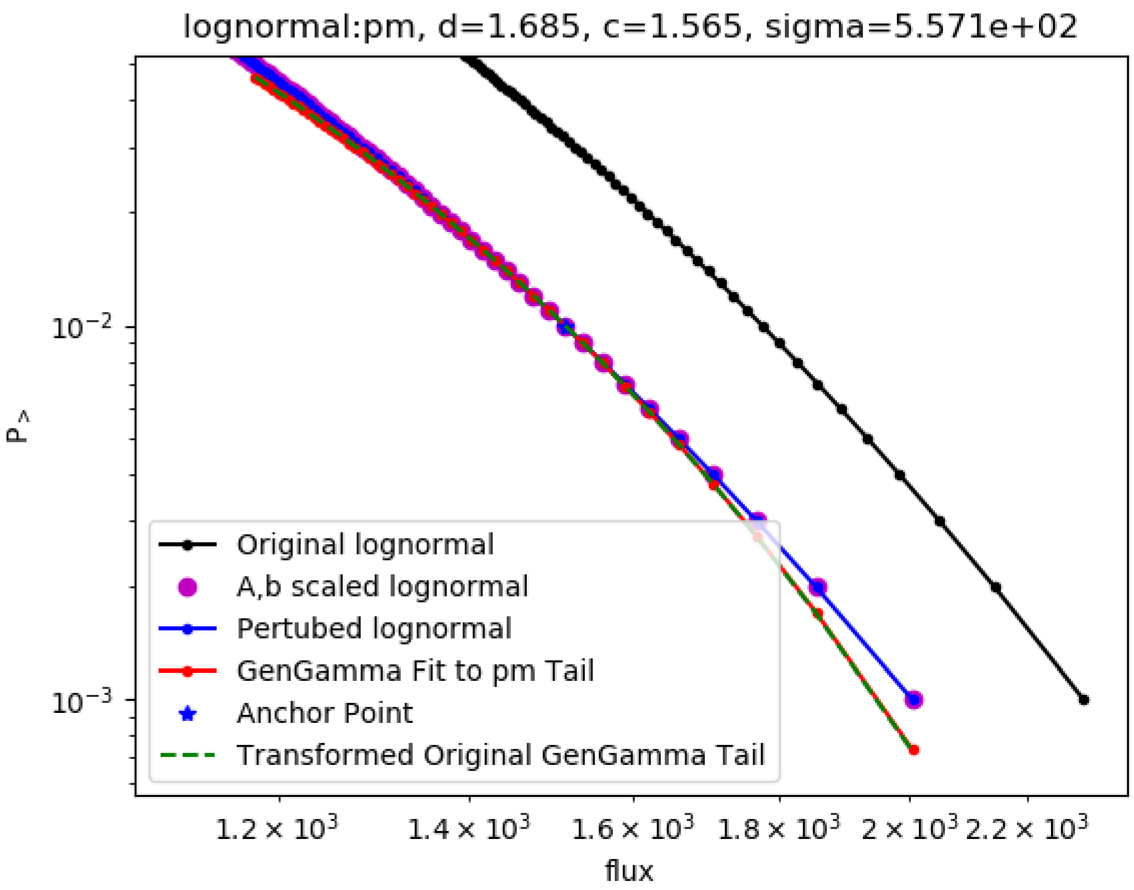
Weibull Example





Log-Normal Example





Summary

- New approach:
  - Provides flux at a fixed set of percentiles
  - Includes a generalized gamma distribution for the right tail
  - Allows power-law perturbation of entire distribution and tail based on perturbing 50^{th} and 95^{th} percentiles
- Improvements
  - Achieves greater accuracy via tabular percentiles
  - Maintains simple uncertainty quantification via errors on 50^{th} and 95^{th} percentile
  - Seamlessly incorporates Weibull and Log-Normal tails in generalized gamma
- To be determined:
  - How to decide which percentiles to measure directly when samples are small, and which ones to extrapolate with a fit
  - How best to fit the tails, especially in bins with few samples
  - How to spatially interpolate/extrapolate tabular values and tail fits
  - Should we be using SPINNs instead?

New Directions

Should we be Using Statistics and Physics Informed Neural Networks?

- Our models now look like this:
  - A spatio-temporal joint probability distribution over time
  - Represents likelihood of flux j at two points $(\vec{x}_i, t_i)$ and $(\vec{x}_k, t_k)$
  - $p\big(j(\vec{x}_i, t_i), j(\vec{x}_k, t_k)\big) = p(j_i; \vec{x}_i)p(j_k; \vec{x}_k)c(j_i, j_k; \vec{x}_i, \vec{x}_k, t_i - t_k)$
  - $p(j; \vec{x}) = \left.\frac{dF}{dj}\right|_{\vec{x}}$ - marginal distribution of flux at $\vec{x}$
  - $c(j_i, j_k; \vec{x}_i, \vec{x}_k, \Delta t)$ – copula describing covariance structure as a function of time lag Δt (C is cumulative copula)
- New developments in neural networks allow us to represent unknown functions F, C as neural networks
- Training could be done on heterogeneous data:
  - Simulation data
  - Unidirectional differential fluxes
  - Integral fluxes
  - Raw sensor counts (accounting for sensor response that integrates over grid)
- Training could include statistical constraints:
  - Marginals F have 0,1 bounds and positive derivative everywhere
  - Integral copulas C have boundary conditions and all positive derivatives everywhere
- Training could include physical constraints:
  - Marginal gradients approximate steady state diffusion equation
  - Marginals obey boundary conditions (loss cone, zero gradient at magnetic equator)

SPINN challenges

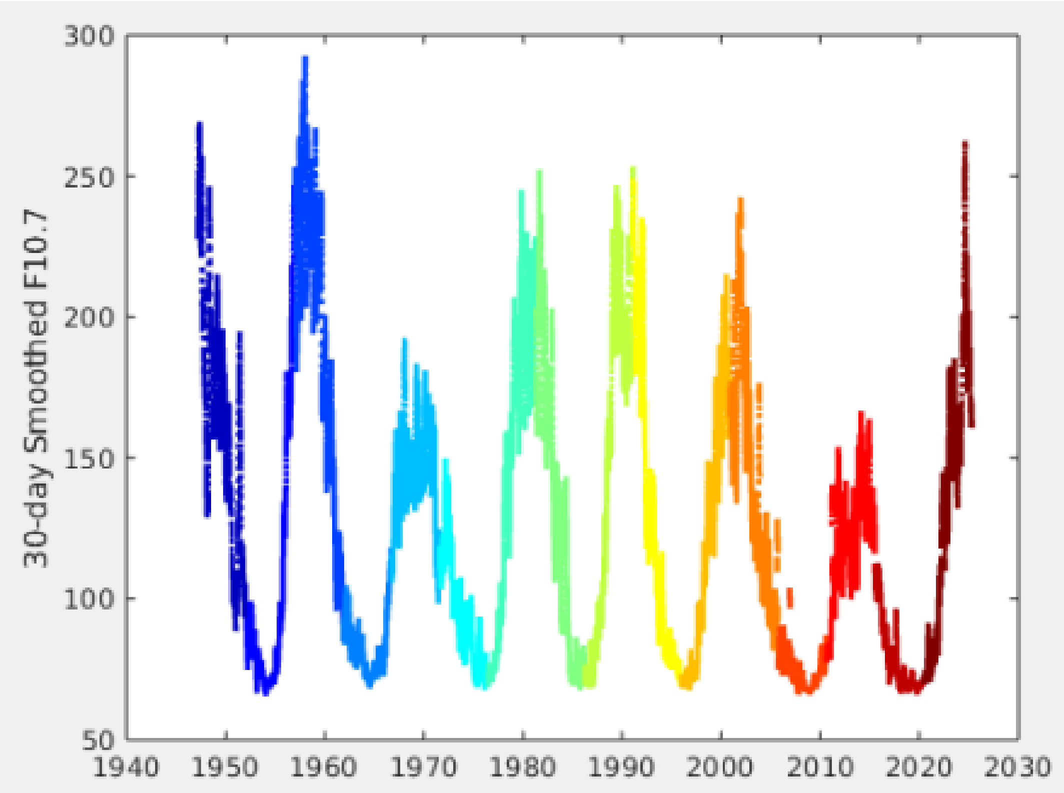
- How do we capture model uncertainty in a SPINN framework? I.e., how do we try to make today's model bound tomorrow's data?
- How do we train a SPINN?
  - Lots of work to figure out how to build penalty functions for legacy data sets
  - Enormous data sets (all flight data ever)
  - Probably some hand tuning to balance data constraints, statistical constraints, physical constraints
- How do we use a trained SPINN?
  - Are we still doing Monte-Carlo sampling to generate scenarios?
  - Will it run quickly enough?
  - Do we need, instead, to use something like cumulants to avoid Monte-Carlo?

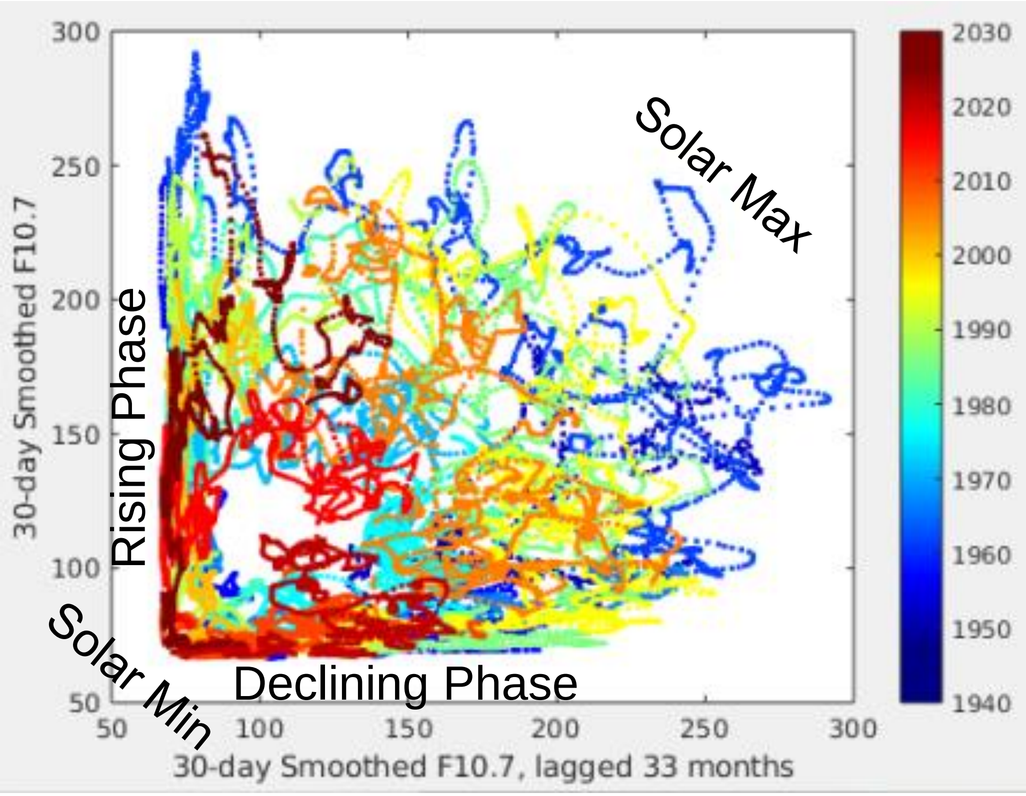
Can we get away from magnetic coordinates?

- One of the computationally expensive and complex pieces of evaluating a radiation environment model is converting from the model's magnetic coordinates to the spacecraft location
- Using principal component compression, we might be able to store everything on a time, altitude, latitude, longitude, energy, pitch-angle grid in a reasonable amount of data
  - ~300 altitude steps from 100 km altitude to R=12 RE. 50 km steps in LEO, ~0.7% dR/R
  - ~100 L/latitude steps, < 3 degrees latitude step, < 0.25 L step
  - 15 longitude steps
  - ~50 energy steps from 1 keV to 1 GeV, 30% dE/E
  - ~10 pitch angle steps (5, 10, 20, … 90 degrees)
  - ~4E8 grid points, stored a single precision (1.6 Gb for unidirectional flux, 0.16 Gb for omni)
- Variation:
  - ~100 principal components (165 Gb for unidirectional flux, 17 Gb for omni)
  - ~300,000 time steps (31 years at 1 hour resolution)
  - 2.7E10 principal component amplitude points
  - ~100 Gb
- Developer interpolates their model onto such a grid before software delivery
- Greatly simplifies delivered software:
  - Computing full flux maps from PCs and amplitudes
  - Interpolating and integrating over flux maps
  - No field model, no field line tracing, no drift shell coordinates
- Does not reduce time for Monte Carlo uncertainty and dynamics

How to parameterize solar cycle variation?

- Solar cycle drives systematic variation in low-altitude proton fluxes (atmospheric density)
- Solar cycle drives systematic variation in the statistics of high-altitude proton and electron fluxes (storms)
- Solar cycles are only quasi-periodic, which poses a challenge for ensuring continuity at solar cycle boundary
- Proposed solution: represent solar cycle phase as two parameters:
  - Current monthly average sunspot number
  - Monthly average sunspot number lagged by ¼ solar cycle (33 months)





Summary

- Neural networks can allow us to define very flexible covariance models
- Covariance NNs can be trained on real and simulation data

- Generalized gamma distribution combined with tabulated percentiles can replace the log-Normal and Weibull formulations we have used previously

- SPINNs might offer a framework to build a grid-free model that can fit heterogeneous data without having to convert everything to unidirectional differential flux

- Principal component compression might allow us to build real-space dynamic maps rather than using magnetic coordinates

- It might be good to parameterize solar cycle dependence in terms of F10.7 and lagged F10.7

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