Using Emulators for Combining Deterministic & Stochastic Models for Hazard Assessment

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A Team Effort...

Along with many current and former students...
Introduction
  The Problem
  Emulation
  Catastrophe Threshold

Combining Deterministic & Stochastic Models

The Stochastic Model
  PF Volumes
    Power Laws
  PF Initiation Angles
  PF Times
  Summary

Results

Extensions
  Improving the Models

Tempering
  Predictions
  Discussion

Conclusions
  Work in Progress
The Caribbean Island of Montserrat
Our Goal:

- Goal: quantify the hazard from Pyroclastic Flows (PFs)—
  - For each location “x” on Montserrat, we would like to find the probability of a “catastrophic event” (e.g., inundation to ≥1m) within $T$ years— for $T = 1, T = 5, T = 10, T = 20$ years. Isoprobability curves ⇒ “Hazard Maps”.
  - Reflecting all that is uncertain, including:
    - How often will PFs of various volumes occur?
    - What initial direction will they take?
    - How will the flow evolve?
    - How are things changing, over time?
    - What are the uncertain model parameters?
  - This is not what is needed for short-term crisis and event management— here we consider only long-term hazard.
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Pieces of the Puzzle

Our team (geologist, volcanologist, applied mathematicians, statisticians, a stochastic processor) breaks the problem down into three parts: two Stochastic, one Deterministic.

- Try to model the volume, frequency, and initial direction of PFs at SHV, based on 15 years' data, using Prob & EVT;
- For specific volume $V$ and initial direction $\theta$ (and other uncertain things like the basal friction angle $\phi$), try to model the evolution of the PF, and max depth $M(x)$ at each $x$, using PDE-based TITAN-2D simulation model
- Try to model what TITAN-2D would say at untried locations, using GP Emulator
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A Brute Force Bayesian Method

• Draw $V_j$, $\tau_j$, $\theta_j$, $\phi_j$ from some dist’n;
• Compute inundation height $M(x; V_j, \theta_j, \phi_j)$ at site $x$ using TITAN-2D for each site $x$ of interest;
• Use M/H to decide if you like the draw;
• Repeat about $10^6$ times
• Consuming about $10^6$ hours.
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- Draw $V_j, \tau_j, \theta_j, \phi_j$;
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Finally, a New Idea

- Key idea: If some volume $V$ with initiation angle $\theta$ inundates location $x$, then any higher volume $V' > V$ will too.
- SO: For each angle $0 \leq \theta < 2\pi$, identify the *smallest* volume $\Psi(\theta; x)$ that will reach $x$.
- Then: Find the probability of at least one $(V_j, \tau_j, \theta_j)$ with:
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- How do we find $\Psi(\theta, x)$?
Emulation

We could pick off $\psi(\theta; x)$ from a grid of TITAN-2D outputs at each of:

- 100 Initiation Angles $\theta_i$;
- 100 Volumes $V_j$;
- 100 Friction Angles $\phi_k$;

Which would entail maybe $100 \times 100 \times 100 = 1,000,000$ runs of TITAN-2D...but we still don’t have 1,000,000 hours. Our Solution:

Build an Emulator for the slow T2D PDE flow model.
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A GP Emulator is a (very fast):

- statistical model (based on Gaussian Processes) for our
- computer model (based on PDE solver) of the
- volcano.

The emulator can predict (in seconds) what TITAN-2D would return (in hours), with an estimate of its accuracy;

Based on Gaussian Stochastic Process (GP) Model. We:

- Pick a few hundred “design points” \((V_j, \theta_j, \phi_j, \ldots)\) (LHD);
- Run TITAN-2D at each of them to find TITAN-2D Model Output \(M(x; V_j, \theta_j, \phi_j)\);
- Train the GP to return a statistical estimate

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A Reminder— What do we Emulate, and Why?

With this we try to evaluate a “threshold function” for each site $x$ in Montserrat:

$$\Psi(\theta; x) = \text{Smallest volume } V \text{ that would inundate site } x \text{ if flow begins in direction } \theta$$

for each possible angle $\theta$ ($0–2\pi$, with $0 = \text{East}$ and $\pi/2 = \text{North}$). Then we Quantify the Uncertain Hazard at $x$ for $T$ years as

$$\text{Pr}\left\{ V_i \geq \Psi(\theta_i; x) \text{ for some PF } (V_i, \theta_i) \text{ in time } (t_0, t_0 + T) \right\}$$

which in turn we study with the probability models.
Finding $\Psi(\theta; x)$ In Pictures
**Designs and Sub-designs**

- We train the **Emulator** at “Design Points” \( \{(V_i, \theta_i, \phi_i)\} \)—
  - Not random variables from a prior distribution— rather,
    - a deliberately chosen set of points, intended to be as widely-dispersed as we can manage in a 3-dim space.

- We use a maxi-min **Latin Hypercube Design** (LHD), with 2048 points in \([10^5, 10^9] \times [0, 2\pi) \times (8^\circ, 12^\circ)\)

- ...but we can’t invert 2048 \times 2048 matrices inside an MCMC loop, so we look for special **SUBDESIGNS** (\(\approx 40–50\) pts) for each \(x\) of the design points **important for that \(x\).**
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Design points $V, \theta$

2048 Design Points total; 40 used for determining $\Psi$ at $x=\text{Level 4 Trigger Point: Dyers River Valley (head of Belham valley)}$. 

Black $\iff M(x; V, \theta, \phi) = 0$ Red $\iff M(x; V, \theta, \phi) > 0$;

$-$: $8^\circ < \phi < 8.5^\circ$; $\bigcirc$: $8.5^\circ < \phi < 10.5^\circ$; $+$: $10.5^\circ < \phi < 12^\circ$.
50 Simulations of $\psi(\theta; x)$ for TP4, Dyers RV
Combining Det & Stoch Models

We have tried to separate our challenge into

- The **Deterministic** problem of identifying those “input values” $V, \theta, \phi$ that lead to a catastrophe at $x$, using T2D, and
- The **Stochastic** problem of finding the probability of such an event.

- Use **Det Model** to identify the Hazard Region in parameter space;
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I say “tried” because we needed to **Emulate** T2D and emulation will entail more uncertainty to combine!!
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SO, we need a joint model for points \(\{(V_j, \theta_j, \tau_j)\} \subset \mathbb{R}^3\).
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PF Volumes

Seems kind of linear, on log-log scale... remember that.
PF Frequencies (1990’s–2010)

- PF’s exceeding $10^4$ m$^3$: Daily, 0–1.6 km runout
- PF’s exceeding $10^5$ m$^3$: Fortnightly, 2–3.0 km runout
- PF’s exceeding $10^6$ m$^3$: Quarterly, 4–6.0 km runout
- PF’s exceeding $10^7$ m$^3$: Yearly, 6.0+ km runout
- PF’s exceeding $10^8$ m$^3$: Just two, unknown runout
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Remember how the log-log *Freq. vs. Volume* plot was nearly linear? Linear log-log plots of *Magnitude vs. Frequency* are a hallmark of the *Pareto* probability distribution $\text{Pa}(\alpha, \epsilon)$,

$$ P[V > v] = (v/\epsilon)^{-\alpha}, \quad v > \epsilon. $$

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Power Laws

Remember how the log-log plot was nearly linear? Linear log-log plots of Magnitude vs. Frequency are a hallmark of the Pareto probability distribution $\text{Pa}(\alpha, \epsilon)$,

$$P[V > v] = (v/\epsilon)^{-\alpha}, \quad v > \epsilon.$$  

Which is kind of bad news.
The Pareto Distribution

The negative slope seems to be about $\alpha \approx 0.64$ or so. The Pareto distribution with $\alpha < 1$ has:

- Heavy tails;
- Infinite mean $E[V] = \infty$, infinite variance $E[V^2] = \infty$;
- No Central Limit Theorem for sums ($\alpha$-Stable instead);
- Significant chance that, in the future, we will see volumes larger than any we have seen in the past. Like $V > 10^9 \text{m}^3$.
- The Pareto comes up all the time in the Peaks over Threshold (PoT) approach to the Statistics of Extreme Events—related to Fisher/Tippett Three Types Theorem.
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How big is bad?

Kinda depends which way it goes...
PF Initiation Angles

Our data on angles is quite vague—we only know which of 7 or 8 valleys were reached by a given PF, from which we can infer a sector but not a specific angle $\theta$:

Any nonuniformity for $\theta$? Any dependence of $\theta$ on Volume $V$?
Angle/Volume Data (cont)

We need a joint density function

\[ f(V, \theta) = f(V) f(\theta | V) \]

given by:

\[ V, \theta \sim \alpha \varepsilon^\alpha V^{-\alpha - 1} 1_{\{V > \varepsilon\}} \pi_\kappa(\theta) \]

where \( \pi_\kappa(\theta) \) is the von Mises distribution with pdf

\[ f(\theta | \kappa, \mu) = \frac{e^{\kappa \cos(\theta - \mu)}}{2\pi I_0(\kappa)} , \]

centered at \( \theta \approx \mu \) close to zero (East) with concentration \( \kappa \) that might depend on \( V \) if the data support that.
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PF Times

If we observe $\lambda$ PFs per year of volume $V > \epsilon$, then what is the probability that such a PF will occur in the next 24 hours? For short-term predictions, it may be important to note this can depend on:

- How high is the dome just now?
- Any seismic activity suggesting dome growth and instability?
- Has it rained recently?
- How long a time interval since last PF?

But, for long-term predictions all these factors average out and we assume that:

- PF occurrences in disjoint time intervals are independent
- PF rates are constant over time, neither rising nor falling.
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Under those assumptions (which we will revisit), the number of PFs in any time interval of length $\Delta t$ (like $1/365$, for a single day) has an expected number of $\lambda \Delta t$ PFs and a probability of

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A Summary of our Stochastic Model:

The data suggest a (provisional!) model in which:

1. PF Volumes are iid from a Pareto $\text{Pa}(\alpha, \epsilon)$ distribution for some shape parameter $\alpha (\approx 0.64)$ and minimum flow $\epsilon (\approx 5 \cdot 10^4 \text{ m}^3)$; and

2. PF Initiation Angles have a von Mises distribution on $[0, 2\pi)$; and

3. PFs arrival times follow a stationary Poisson process at some rate $\lambda (\approx 22)/\text{yr}$.

These have the beautiful and simplifying consequence that the number of PFs in any region of three-dimensional ($V \times \theta \times \tau$) space has a Poisson probability distribution—so, we can evaluate:
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The hazard prediction we wish to make is

\[
P[ \text{Catastrophy within } t \text{ Years }] = 1 - P[Y_t = 0] \quad (\text{where } Y_t \text{ is the number of catastrophes})
\]

\[
= 1 - \exp\left(-EY_t\right)
\]

\[
= 1 - \exp\left(-t \lambda_\varepsilon \int_{V > \Psi(\theta;x)} \varepsilon^\alpha \alpha V^{-\alpha-1} dV \pi_\kappa(d\theta)\right)
\]

Which we can compute pretty easily on a computer:
If we knew the (uncertain) values of the Pareto parameter $\alpha \approx 0.64$, rate parameter $\lambda_\epsilon \approx 22/\text{yr}$, basal friction $\phi \approx 8-11^\circ$. 
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The necessary integrals in $V$ and $\lambda_\epsilon$ are available in closed form; we accommodate (posterior uncertainty) about $\alpha$ and $\phi$ using MCIS.
Computing the Posterior

\[ P[ \text{Catastrophy within } t \text{ Years } | \lambda_\epsilon, \alpha, \phi] \]

\[ = 1 - \exp \left( -t \lambda_\epsilon \int_{V > \psi(\theta; x)} \epsilon^{\alpha} \alpha V^{-\alpha - 1} dV \, \pi_{\kappa}(d\theta) \right) \]

\[ = 1 - e^{-t \lambda_\epsilon I_\epsilon(\alpha, \phi)} \quad \text{where} \quad I_\epsilon(\alpha, \phi) = \int_0^{2\pi} \left\{ \frac{\psi(\theta; x)}{\epsilon} \right\}^{-\alpha} \pi_{\kappa}(d\theta) \]

\[ P[ \text{No Catastrophy } | \text{ Data } ] \]

\[ = Z^{-1} \int e^{-t \lambda_\epsilon I_\epsilon(\alpha, \phi)} L(\alpha, \lambda, \phi) \pi(d\lambda d\alpha d\phi) \]

\[ = Z^{-1} \int \left\{ 1 + \frac{t}{Tb} I_\epsilon(\alpha, \phi) \right\}^{-J_\epsilon - a} L(\alpha, \phi) \pi(d\alpha d\phi) \]

\[ \approx \frac{1}{N} \sum \left\{ 1 + \frac{t}{Tb} I_\epsilon(\alpha_i, \phi_i) \right\}^{-J_\epsilon - a} \]
Computing the Posterior

\[ P[ \text{No Catastrophy} \mid \text{Data}] \]

\[ = \frac{1}{Z} \int e^{-t \lambda e l_e(\alpha, \phi)} L(\alpha, \lambda, \phi) \pi(d\lambda d\alpha d\phi) \]

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Hazard Over Time at Plymouth & Bramble

\[ P(t) = P[ \text{Catastrophe in t yrs} \mid \text{Data} ] \]
Hazard Over Space, for 2.5 Yrs
A few more Hazard Maps

Probability Contours: 0.1, 0.5, 0.9

1. Furthest extent of flows to date
2. Level 4 trigger
Current Official Hazard Map...
Extensions & Related matters...

Some challenges along the way:

▶ TITAN-2D relies on Digital Elevation Models for its flow predictions. How can we quantify uncertainty in the DEM and its effect on hazard?

▷ Our team is building “elastic” models, in collaboration with UB geologist Beá Csathó;

▶ MVO is a spectacular and rare resource, giving unrivaled wealth of data for SHV. How can we use Seismic Data at other volcanoes to improve hazard prediction?

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Model Improvements Underway

All three of our Preliminary Assumptions are wrong, of course:

1. PFs arrive as stationary Poisson proc. at rate $\lambda(\approx 22)/\text{yr}$;

In fact the rate $\lambda_t$ varies over time, and sometimes seems to vanish for a while at times. We’re building dynamic models for this, which feature possibility of $\lambda_t = 0$ for some time intervals.

No cyclicity yet (7–11 hr, 6–7 wk, etc.),
No dynamic changes in $\theta$ dist’n,
No Survival Curve (yet!).
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We’ve already seen signs that easterly flows are more frequent, and suggestions that $V$ and $\theta$ may be dependent. Can extend to mixture of von Mises, regression model, etc. Probably I’m out of time now, and it’s time to Wrap Up; if not, I’ll show how we’re approaching one of these issues:
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Tempered Pareto Models

There’s a slight suggestion of a *downturn* in the Freq-vs-Vol log-log plot; perhaps a better model is **Tempered Pareto**, with

\[
P[V > v] = \left(\frac{v}{\epsilon}\right)^{-\alpha} e^{-\beta(v-\epsilon)}, \quad v > \epsilon:
\]

Tempered Pareto TP(\(\alpha = 0.43, \epsilon = 10^4, \kappa = 10^{10}\)) Distribution

See the drop-off near \(10^8 \text{ m}^3\) or \(10^9 \text{ m}^3\)? That's Good news!
Tempered Pareto Models

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Uncertainty

MLE and reference Bayesian posterior means (± SD’s) for the three parameters of this model are:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mean</th>
<th>± SD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shape ( \alpha )</td>
<td>( \approx 0.64 \pm 0.04 )</td>
<td></td>
</tr>
<tr>
<td>Rate ( \lambda )</td>
<td>( \approx 22.42 \pm 1.3 ) /year</td>
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Note how uncertain \( \beta \) is... only 1.5 SD above zero.
How does this affect hazard predictions?
How does Pareto (\( \beta = 0 \)) model differ from Tempered Pareto (\( \beta > 0 \))?
Uncertainty

MLE and reference Bayesian posterior means (± SD’s) for the three parameters of this model are:

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Hazard for Fifty Years of $V > 10^8 \text{ m}^3$

Risk Comparisons, Tempered vs. Untempered Zipf, for $\Psi = 10^8 \text{ m}^3$
Hazard for Fifty Years of $V > 5 \times 10^8 \text{ m}^3$

Risk Comparisons, Tempered vs. Untempered Zipf, for $\Psi = 5 \cdot 10^8 \text{ m}^3$
Why the wide uncertainty?
How does that affect estimated hazard?

Risk for $\Psi = 5 \cdot 10^8$ m$^3$

Temp. Pareto model:

$E\alpha = 0.63$, $E\beta^{-1} = 10^{8.04}$ m$^3$
What if there is no tempering?

Risk for $\Psi = 5 \cdot 10^8$ m$^3$

Untemp. Pareto model: $E\alpha = 0.64$
A little more extreme—Truncated Pareto

\[
P[V > v] = \frac{v^{-\alpha} - L^{-\alpha}}{\epsilon^{-\alpha} - L^{-\alpha}} \quad \epsilon \leq v \leq L:\]

Now the drop-off approaching \(10^9\) m\(^3\) is fast!
A little more extreme—Truncated Pareto

![Graph showing annual rate against PF volume for Truncated Pareto distribution.]
A little more extreme—Truncated Pareto

Risk for \( \Psi \equiv 10^8 \text{ m}^3 \)

Trunc. Pareto model:

\( E\alpha = 0.63, \quad EL = 10^{8.98} \text{ m}^3 \)

Prior \( L \approx \text{Ga}(1, 1e^{-09}) \)
Morals

- It’s hard to tell about tail behaviour (extremes) from data;
- Clearer picture of tempering would help—working to elicit expert opinion about physical limits;
- All our model assumptions benefit from closer scrutiny.
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• Clearer picture of tempering would help—working to elicit expert opinion about physical limits
• All our model assumptions benefit from closer scrutiny.
Conclusions

- Probability, Statistics, Computational PDE, and physical Sciences (Geo, Phys, Ast, Bio, Chem, ...) are a good mix!
- Useful to **Separate** the **Stochastic & Deterministic** aspects
  - Use **Deterministic** models to identify region $\mathcal{R}_C$ of input parameter space for **Catastrophes**
  - Use **Stochastic** models to identify posterior probability

$$P[\mathcal{R}_C | \text{Data }]$$
Ongoing Work & Extensions

• Studying dynamic models for variable rate of eruption process and changing direction of flows ($\Rightarrow$ short-term predictions);

• Exploring dependence between angle $\theta$ and flow volume $V$;

• Estimating possible “tempered Pareto” models,

  \[ P[V > v] = \left(\frac{v}{\epsilon}\right)^{-\alpha} e^{-\beta(v-\epsilon)}, \quad v > \epsilon \]

• Non-stationary variants;

• Finite lifetimes (“dormancy” and “extinction”).
Thanks!

More details (references, this talk in .pdf, related work) are available on request from

rlw@duke.edu.

Thanks to SAMSI, SIAM, MVO and to the NSF\textsuperscript{1}!

\textsuperscript{1}ACI-1550225, DMS-0757549, DMS-1228317, DMS-1622403, SES-1521855.