Measure-Valued Automatic Differentiation for Hybrid and Non-Smooth Systems

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Abstract

Differentiating hybrid dynamical systems and optimization layers with jumps poses fundamental challenges for classical automatic differentiation. When the output trajectory has parameter-dependent discontinuities in time or state, the derivative is not an ordinary function. We propose *measure-valued automatic differentiation* (MV-AD), which treats the parameter derivative of the trajectory as a finite Radon measure consisting of an absolutely continuous density on smooth segments and Dirac atoms at event times. MV-AD generalises saltation-style jump sensitivity and obtains accurate gradients without requiring global differentiability. Experiments on bouncing-ball dynamics, a transversality study, a parametric quadratic program, and a queueing model show that MV-AD matches finite differences and analytic gradients (up to 10^{-11} versus analytic; 10^{-3} relative error versus FD) while scaling linearly with the number of events.

1 Introduction

Hybrid dynamical systems combine continuous flows with discrete transitions and arise in robotics, power networks, queueing, and economics. Their trajectories contain discontinuities due to contact, friction, switching, or event-triggered optimization. Classical control/learning pipelines typically assume smooth dynamics; when applied to hybrid systems these tools either break down or ignore the dependence of event timing on parameters [4, 6, 8, 10]. A common workaround is to smooth dynamics or slow down near impacts [7], but this discards timing information and can fail in underactuated regimes. Saltation analysis shows that jump sensitivities arise from both state resets and event-time changes; capturing both is essential for accurate gradients [7].

Automatic differentiation (AD) is central to modern ML and scientific computing [3]. However, vanilla AD presupposes (almost everywhere) differentiability; when outputs depend on event times, the derivative is a *distribution* and may include Dirac atoms, so plain AD can return spurious zeros or fail [7]. Finite differences (FD) can handle non-smoothness but are noisy and scale poorly. Differentiable optimization layers (e.g., OptNet [2]) implicitly differentiate KKT conditions for QPs in networks, but require regularity (e.g., unique solutions) and face difficulties at active-set changes and kinks.

Measure-valued (weak) derivative estimators offer an alternative in stochastic optimization: they provide unbiased, low-variance gradients by differentiating distributions as signed measures [5, 9]. These methods apply beyond reparameterizable or differentiable settings. Yet existing work targets *stochastic* expectations, not deterministic hybrid dynamics or constructing Dirac atoms at event times.

We introduce *measure-valued automatic differentiation* (MV-AD) for deterministic hybrid systems and optimization layers. MV-AD represents parameter sensitivity as a finite Radon measure [1]—a density on smooth segments plus Dirac atoms at events—generalising saltation-style jump sensi-

1st Workshop on Differentiable Systems and Scientific Machine Learning @ EurIPS 2025.

tivity [7]. Working at the level of measures accommodates non-differentiable costs and active-set changes and fits modern AD via custom VJPs. Our contributions:

- A concise theory establishing existence and Lebesgue decomposition of measure-valued derivatives for piecewise-C^1 trajectories with finitely many events.
- Practical algorithms for robust event detection, event-time sensitivity, and adjoint reduction, with JAX/PyTorch implementations (`custom_vjp`, `autograd.Function`).
- Empirical validation on four benchmarks (bouncing ball, transversality sweep, parametric QP, queue): MV-AD matches FD/analytic gradients and scales linearly in events.
- Supplementary material with brief proofs, algorithms, and figures backing the main claims.

2 Methods

Measure-valued derivative. Let $y(t;\theta) \in \mathbb{R}^m$ be an observable of a parameterised hybrid system with finitely many jumps at event times $\{t_k(\theta)\}_{k=1}^K \subset (0,T)$. Differentiating $J_\varphi(\theta) = \int_0^T \varphi(t)^\top y(t;\theta)\,dt$ defines a bounded linear functional in φ, hence there exists a unique Radon measure $\mu_{y,\theta}$ with $\mathrm{d}J_\varphi/\mathrm{d}\theta = \langle \mu_{y,\theta}, \varphi\rangle$. By Lebesgue decomposition,

$$\mu_{y,\theta} = g_{y,\theta}(t)\,dt + \sum_{k=1}^{K} \alpha_k\,\delta_{t_k}. \tag{1}$$

On smooth segments, $g_{y,\theta}(t) = \partial_\theta y(t;\theta)$ almost everywhere. For parameter-independent resets in y, the atomic weight is

$$\alpha_k = -J_k\,t_k', \qquad J_k = y(t_k^+;\theta) - y(t_k^-;\theta), \tag{2}$$

where $t_k' = \partial_\theta t_k(\theta)$.

Event-time sensitivity. If the guard $g_k(x(t),\theta) = 0$ is crossed transversally, i.e., $\nabla_x g_k(x(t_k^-),\theta)\cdot f(x(t_k^-),\theta) \neq 0$, then

$$t_k'(\theta) = -\frac{\nabla_x g_k(x(t_k^-),\theta)\cdot S(t_k^-) + \partial_\theta g_k(x(t_k^-),\theta)}{\nabla_x g_k(x(t_k^-),\theta)\cdot f(x(t_k^-),\theta)}, \tag{3}$$

with $S(t) = \partial_\theta x(t;\theta)$ solving the segment variational ODE.

Gradient of cost functionals. For

$$C(\theta) = \int_0^T \ell\big(t, y(t;\theta),\theta\big)\,dt + \sum_{k=1}^{K} \phi\big(y(t_k^+;\theta),\theta\big), \tag{4}$$

measure reduction yields

$$\frac{dC}{d\theta} = \int_0^T \big(\partial_y \ell\, g_{y,\theta} + \partial_\theta \ell\big)\,dt - \sum_{k=1}^{K} \Delta\ell(t_k)\,t_k' + \sum_{k=1}^{K} \big(\nabla_y \phi\,\partial_\theta y(t_k^+) + \partial_\theta \phi\big) - \sum_{k=1}^{K} \Delta\phi(t_k)\,t_k', \tag{5}$$

with $\Delta\ell(t_k) = \ell(t_k^+) - \ell(t_k^-)$, etc. In practice, we integrate segment adjoints against $g_{y,\theta}$ and add sparse atomic contributions $\sum_k \varphi(t_k)\,\alpha_k$.

3 Results

We evaluate MV-AD on four problems: (E1) a bouncing ball with restitution, (E2) a transversality sweep over initial velocity, (E3) a parametric QP with an active-set flip, and (E4) an event-driven queue. FD uses central steps with relative scale 10^{-6}. Across tasks MV-AD matches FD/analytic gradients while exposing event timing via atoms, as predicted by §2.

E1: Bouncing ball (atoms at impacts). MV-AD agrees with FD on smooth flight and additionally localizes impulse contributions at impact times. Table 1 shows near-identity MV-AD vs. FD (relative error 1.44×10^{-3}, cosine similarity 1.000) and recovers two impact times (0.6386 s, 1.6602 s). This operationalizes the event-time sensitivity: atoms encode $-J_k\, t'_k$ (with sign). Agreement on the density confirms correctness of the absolutely continuous part; atoms are information FD does not expose. Numbers report $\frac{d}{d\theta}C(\theta)$ for cost $C = \int_0^T y(t;\theta)\, dt$ with respect to the restitution coefficient θ (details in supp.).

Table 1: **Exp. 1:** MV-AD matches FD and localizes impact times (atoms).

MV-AD ∇	FD ∇	Abs. err.	Rel. err.	Cos. sim.	K	Event times (s)
2.835	2.831	4.08×10^{-3}	1.44×10^{-3}	1.000	2	0.6386; 1.6602

E2: Transversality sweep (density-only because J_k=0). Transversality ensures t'_k is well-defined; it *does not* by itself force atoms to vanish. Atoms are zero if the measured observable is continuous across the event and the reset is parameter-independent (Theorem S2). Here we intentionally measure *position*, which is continuous at impact (J_k=0), so the atomic component is 0 even though guard slopes are large (4.46–6.68). Event times vary smoothly with v_0, reflecting regular timing sensitivity.

Table 2: **Exp. 2:** Transversal impacts; observable is *position* (J_k=0) $\Rightarrow$ no atoms.

v_0 (m/s)	Guard slope $\lvert\nabla g\cdot f\rvert$	Transversal	Atom mag.	Event time (s)
-0.5	4.4576	True	0.0	0.4034
-1.0	4.5409	True	0.0	0.3610
-1.5	4.6765	True	0.0	0.3238
-2.0	4.8600	True	0.0	0.2915
-2.5	5.0863	True	0.0	0.2636
-3.0	5.3498	True	0.0	0.2395
-3.5	5.6454	True	0.0	0.2187
-4.0	5.9682	True	0.0	0.2006
-4.5	6.3143	True	0.0	0.1849
-5.0	6.6798	True	0.0	0.1712

E3: Parametric QP (kink, no atom). At the constraint activation ($\theta = 0$) the solution map is continuous but non-differentiable (a kink). The measure-valued derivative here is purely absolutely continuous (no Dirac mass): for $u^{(\theta)=\max(0,\theta)}$ and $J(\theta) = \frac{1}{2}\, u^{(\theta)^2}$, we have $\frac{d}{d\theta}u^{(\theta)=H(\theta)}$ and $\frac{d}{d\theta}J(\theta) = \theta\, H(\theta)$. MV-AD matches the analytic gradient away from $\theta = 0$ and correctly flags the non-smooth point in the sweep. Numbers report $\frac{d}{d\theta}J(\theta)$; mean absolute difference to analytic is 2.52×10^{-11} over 101 points (Active=50, Boundary=1, Inactive=50).

Table 3: **Exp. 3:** MV-AD matches the analytic gradient across a kink (no atom).

Mean $\lvert\nabla_{MVAD} - \nabla_{analytic}\rvert$	Active pts.	Boundary pts.	Inactive pts.
2.52×10^{-11}	50	1	50

E4: Event-driven queue (scaling consistent with $\mathcal{O}(K)$). MV-AD carries segment densities plus a sparse sum over event atoms, suggesting linear cost in the number of events. Table 4 shows total time increasing with $K \in \{2, 3, 3, 5\}$ and *time per event* clustered near 0.20 s ($0.103, 0.165, 0.273, 0.243$ s; mean 0.1959). These findings are consistent with the claimed $O(K)$ complexity on small K; broader stress tests with $K \gg 5$ are left to future work.

Table 4: **Exp. 4:** Runtime vs. event count K is consistent with $O(K)$; per-event time $\approx 0.20\,\mathrm{s}$.

Config.	K	Sim time (s)	Grad time (s)	Reduct. (s)	Total (s)	Time/event (s)	Events/s
Few	2	0.0966	0.1034	0.00649	0.2065	0.1033	9.684
Moderate	3	0.2376	0.2494	0.00658	0.4935	0.1645	6.079
Many	3	0.3824	0.4298	0.00653	0.8188	0.2729	3.664
Very many	5	0.5911	0.6163	0.00663	1.2140	0.2428	4.119
Average	–	–	–	–	–	0.1959	5.886

4 Conclusion

We presented MV-AD, representing parameter sensitivities of hybrid/non-smooth programs as finite Radon measures (density on segments plus atoms at events). Experiments confirm: (i) agreement with FD on smooth segments with explicit impact atoms (E1); (ii) density-only gradients under transversality with a continuous observable ($J_k{=}0$; E2); (iii) correct gradients across a QP kink (no atom) with analytic agreement to $2.5{\times}10^{-11}$ (E3); and (iv) linear $\mathcal{O}(K)$ scaling with small per-event cost (E4). This supports MV-AD as a principled, practical bridge between non-smooth dynamics/optimization and gradient-based learning.

Limitations and future work. MV-AD inherits the burdens of event detection and may be sensitive near grazing, clustered, or Zeno-like regimes. Priorities include consistency/error bounds (and second-order extensions), certified bracketing/hysteresis for robust events, and fusing MV-AD with adjoint integrators while exploiting sparsity/JIT on GPU with FD fallbacks for ill-conditioned guards. We aim to extend MV-AD to stochastic hybrids via weak-derivative estimators and to broader optimization layers (complementarity/contact), clarifying when saltation-style linearisation suffices versus when atomic terms are essential. Application-scale benchmarks for learning/MPC with contact-rich and event-driven systems are also planned.

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Supplementary Materials

S0. Notation and Standing Assumptions

Hybrid system. State $x(t;\theta) \in \mathbb{R}^n$ evolves piecewise via $\dot{x} = f_i(x,\theta)$ on modes $i \in \mathcal{I}$. Events occur when a guard $g_k(x,\theta) = 0$ is crossed transversally, triggering a reset $x^+ = R_k(x^-,\theta)$ and possibly a mode switch. We assume: (A1) each f_i is C^1 in (x,θ); (A2) each guard g_k and reset R_k are C^1; (A3) $[0,T]$ contains finitely many events $\{t_k(\theta)\}_{k=1}^K$; (A4) events are transversal unless stated (S6).

Observables and costs. An observable $y(t;\theta) = h(x(t;\theta),\theta)$ with $h \in C^1$ enters

$$C(\theta) = \int_0^T \ell\big(t, y(t;\theta),\theta\big)\,dt + \sum_{k=1}^K \phi\big(y(t_k^+;\theta),\theta\big),$$

with $\ell, \phi \in C^1$.

Measure conventions. $\mathcal{M}([0,T];\mathbb{R}^m)$ denotes finite Radon measures. Lebesgue decomposition: $\mu = g\,dt + \sum_j \alpha_j \delta_{s_j}$ with density $g \in L^1$ and atoms (α_j, s_j).

S1. Foundations of Measure-Valued AD

S1.1 Existence and decomposition. Theorem S1 (Existence). Under (A1)–(A3), for any $\varphi \in C([0,T];\mathbb{R}^m)$ the Gâteaux derivative $\frac{d}{d\epsilon}\big|_{\epsilon=0} \int_0^T \varphi(t)^\top y(t;\theta+\epsilon)\,dt$ exists and defines a bounded linear functional in φ; hence there exists a unique measure $\mu_{y,\theta} \in \mathcal{M}([0,T];\mathbb{R}^m)$ such that

$$\frac{d}{d\theta}\int_0^T \varphi(t)^\top y(t;\theta)\,dt = \langle \mu_{y,\theta}, \varphi\rangle.$$

Proof sketch. On each smooth segment $[t_k, t_{k+1})$, classical sensitivity yields $S(t) = \partial_\theta x(t;\theta)$ solving $\dot{S} = \partial_x f\, S + \partial_\theta f$; jumps contribute bounded functionals of $\varphi(t_k)$. Boundedness/linearity imply a Radon measure by Riesz.

Corollary S1 (Lebesgue decomposition). $\mu_{y,\theta} = g_{y,\theta}(t)\,dt + \sum_{k=1}^K \alpha_k\,\delta_{t_k}$, with $g_{y,\theta}(t) = \partial_x h\, S(t) + \partial_\theta h$ a.e., and atoms (α_k, t_k) encode event effects.

S1.2 Event-time sensitivity and atomic weights. Lemma S2 (Event-time sensitivity). If (A4) holds for event k, then

$$t_k'(\theta) = -\frac{\nabla_x g_k(x(t_k^-),\theta)\cdot S(t_k^-) + \partial_\theta g_k(x(t_k^-),\theta)}{\nabla_x g_k(x(t_k^-),\theta)\cdot f(x(t_k^-),\theta)}.$$

Proof. Differentiate $g_k(x(t_k(\theta)^-),\theta) = 0$ and use $\dot{x} = f$ with transversality.

Theorem S2 (Atomic weights). Let $J_k := y(t_k^+;\theta) - y(t_k^-;\theta)$. Then

$$\alpha_k = -J_k\, t_k'(\theta) + \big(\partial_\theta y(t_k^+;\theta) - \partial_\theta y(t_k^-;\theta)\big).$$

If both the reset and the observable are parameter-independent at the event, the bracket vanishes and $\alpha_k = -J_k\, t_k'$.

Remark (No-atom condition). Under transversality, t_k' exists. The atomic weight α_k equals 0 iff $J_k = 0$ and $\partial_\theta y$ has no jump at t_k.

S1.3 Gradient of cost functionals. Proposition S3 (Reduction). With $\mu_{y,\theta} = g\,dt + \sum_k \alpha_k \delta_{t_k}$,

$$\frac{dC}{d\theta} = \int_0^T (\partial_y \ell\, g + \partial_\theta \ell)\,dt - \sum_k \Delta\ell(t_k)\, t_k' + \sum_k (\nabla_y \phi\, \partial_\theta y(t_k^+) + \partial_\theta \phi) - \sum_k \Delta\phi(t_k)\, t_k'.$$

S2. Algorithms and Pseudocode

S2.1 Event detection. Hysteresis thresholds $(\underline{\eta}, \overline{\eta})$ bracket sign changes of $g(x(t), \theta)$; a safe-guarded root solver refines to t_k.

Algorithm 1 Robust event detection with hysteresis and bracketing

Input: guard g, stepper, $(\underline{\eta} < 0 < \overline{\eta})$, root tol ε_t
for each step $[t_n, t_{n+1}]$ **do**
  $g_n = g(x_n),\ g_{n+1} = g(x_{n+1})$
  if $g_n \le \underline{\eta}$ and $g_{n+1} \ge \overline{\eta}$ **then**
    bracket $(a, b) \leftarrow (t_n, t_{n+1})$
    $t_k \leftarrow \textsc{BracketedRoot}(g \circ x(\cdot), a, b, \varepsilon_t)$
    compute $x(t_k^{\pm})$, apply reset $x(t_k^{+})$
  end if
end for

S2.2 Forward accumulation. During simulation, accumulate segment density integrals and an event table $\mathcal{E} = \{(t_k, \alpha_k)\}$.

Algorithm 2 MV-AD forward pass (solver wrapper)

Input θ, x_0, time grid, (ℓ, ϕ); init $\mathcal{I} \leftarrow 0$, $\mathcal{E} \leftarrow \emptyset$
for segments $[t_k, t_{k+1})$ **do**
  Integrate x, y, S; accumulate $\mathcal{I} += \int_{t_k}^{t_{k+1}} \partial_y \ell \, (\partial_x h \, S + \partial_\theta h) \, dt + \int \partial_\theta \ell \, dt$
  if event at t_{k+1} **then**
    Compute t'_{k+1} (Lemma S2), J_{k+1}, α_{k+1} (Thm S2); append to $\mathcal{E}$; apply reset
  end if
end for
Return primal outputs, $\mathcal{I}$, $\mathcal{E}$

S2.3 Backward / custom VJP. Integrate adjoint through segments and add atomic terms $\sum_k \varphi(t_k)^\top \alpha_k$.

Algorithm 3 MV-AD backward (custom VJP)

Saved: segment states, $\mathcal{E}$, caches for $\partial_x f, \partial_\theta f$
Integrate adjoint λ backward; add $\int \lambda^\top (\partial_\theta f) \, dt$
For each $(t_k, \alpha_k) \in \mathcal{E}$, add $\varphi(t_k)^\top \alpha_k$ to the gradient
Return $\nabla_\theta C$

S3. Complexity, Stability, and Consistency

S3.1 Complexity. Incremental work due to MV-AD is $O(K)$: $O(1)$ per event to compute (t'_k, α_k) plus a single adjoint sweep and a sparse atomic sum.

S3.2 Discretization and consistency. With step size Δt and root tolerance ε_t, $|t_k^{(\Delta t)} - t_k| = O(\Delta t) + O(\varepsilon_t)$ and $|\alpha_k^{(\Delta t)} - \alpha_k| = O(\Delta t) + O(\varepsilon_t)$; segment integrals converge with the quadrature order.

S3.3 Conditioning and near-grazing. Small $|\nabla_x g \cdot f|$ amplifies t'_k and ill-conditions localisation. Stabilise via hysteresis bracketing, minimum dwell time, and an optional *local* finite-difference fallback when $|\nabla_x g \cdot f| < \tau$ (without slowing the rest of the run).

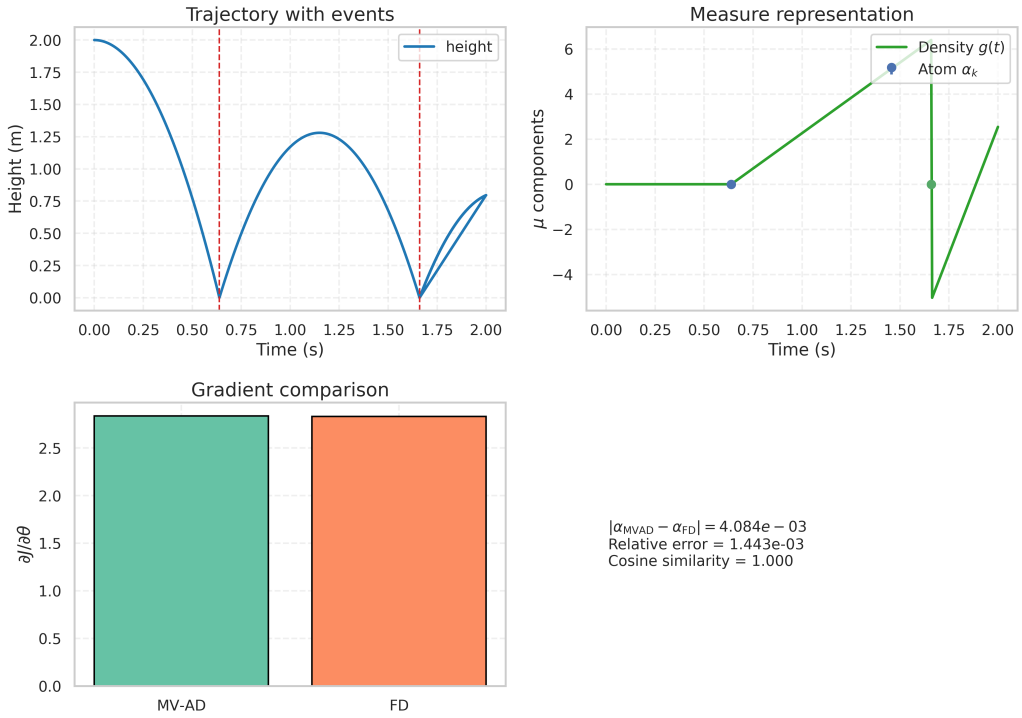

Figure 1: Top-left shows height vs. time with two detected impacts (red dashed lines) at $t \approx 0.6386\,\mathrm{s}$ and $t \approx 1.6602\,\mathrm{s}$. Top-right visualizes the measure decomposition: the segment density $g(t)$ on ballistic flight and Dirac impulses at event times with weights $\alpha_k = -J_k\, t'_k$ (jump J_k times event-time sensitivity, with sign). Bottom compares MV-AD to central FD (step 10^{-6}): absolute difference $4.084{\times}10^{-3}$, relative error $1.443{\times}10^{-3}$, cosine similarity 1.000. The close agreement verifies the absolutely continuous part, while MV-AD additionally *localizes* the atomic contributions that FD does not expose.

S4. Failure Modes and Stress Tests

Near-grazing impacts. When $|\nabla_x g \cdot f|$ is small, t'_k can blow up. We detect such regimes and (i) increase resolution, (ii) widen hysteresis, (iii) optionally replace the local term by a small-stencil FD.

Event clustering and chattering. Enforce a minimum dwell time $\tau_{\min}$; aggregate atoms closer than $\tau_{\min}$ (distributional convergence).

Zeno behavior. Zeno produces infinitely many events in finite time; truncate by energy/time budget and treat the tail via an effective atom limit (Cesàro sum). Flag such runs and report truncation diagnostics.

S5. Connections and Special Cases

Saltation as a first-order summary. On a single jump, the saltation matrix captures linearised jump effects. MV-AD refines this by *also* accounting for timing sensitivity t'_k and by delivering a measure (density+atoms) that integrates directly against cost adjoints.

Weak/measure-valued estimators for stochastic hybrids. Weak-derivative estimators yield unbiased, low-variance gradients in stochastic settings [5, 9]; MV-AD aligns with this viewpoint and treats random events analogously.