# Simultaneous Learning of Control Signals, Parameters, and Model Structure

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Data-driven methods for approximating the underlying dynamics of 1 a complex system have emerged in many different fields of science 2 and engineering. Many approaches posit an autonomous model for 3 the dynamics, such that in the limit of no noise the future state of 4 the system is predictable entirely by its past. Several established 5 methods, such as Dynamic Mode Decomposition (DMD) and Sparse 6 Identification of Nonlinear Dynamics (SINDy), have achieved great success in simultaneously predicting the structure of unknown dy-8 namical systems and their parameter values in autonomous systems. 9 However, many systems of interest, particularly in biology and neuro-10 science, are connected to an outside environment and thus are not 11 autonomous, and in many cases the stimulation is completely un-12 known. We propose an extension of these established methods for 13 simultaneously learning an external control signal along with model 14 structure and parameter values. This requires first extending the 15 methods to a Bayesian framework, and successfully separates the 16 underlying dynamical systems and control signals even in chaotic 17 and noisy? systems. 18

#### 1. Introduction

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Data-driven methods for analyzing complex high-dimensional 2 systems have become very popular, and a goal is often to 3 find an interpretable set of governing equations. These data-4 driven methods generally try to find an autonomous model for 5 the dynamics, for example the recently developed Dynamic 6 Mode Decomposition (DMD) which finds the best-fit linear 7 model along with a low-dimensional set of basis functions, or 8 Sparse Identification of Nonlinear Dynamics (SINDy), which 9 similar but allows nonlinear terms. That is, they posit that the 10 governing equations can be written as a differential equation 11 of the form:  $\dot{\mathbf{x}} = f(\mathbf{x})$ . However, many systems of interest are 12 connected to the outside world, have unmeasured degrees of 13 freedom, or contain dynamics faster than can be measured. 14 An example with a particularly large number of unmeasured 15 variables is that of experimental neuroscience, where in general 16 only a small portion of the brain can be measured. Thus in 17 practice, the dynamics of the observed portion of the system 18 are not autonomous, and appear to be forced by an outside 19 "control signal," "forcing term," or "exogenous shock" that can 20 be written as: 21

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \delta(t) + \epsilon(t)$$
[1]

where f(x) are intrinsic dynamics of interest,  $\delta(t)$  is an unknown discrepancy, and  $\epsilon(t)$  is white noise.

25 The original DMD algorithm (1) was proposed by Schmidt for approximating autonomous, low-dimensional 26 spatio-temporal dynamics in high-dimensional fluids. It was 27 subsequently used in a wide variety of application areas includ-28 ing computer vision (2, 3), neuroscience (4), disease model-29 ing (5), finance (6), and fluid dynamics (1, 7-9). Control was 30 added to produce DMD with control (DMDc) (10, 11), which 31 has an equivalent mathematical form to Eq. 1. Taking the ex-32 ternal control signal into account allowed for both a drastically 33

lower number of relevant dimensions and increased accuracy of the recovered autonomous dynamics. Similar benefits were realized in adding control to nonlinear systems (12). However, these control signals must be known in advance, which is often not the case for natural systems.

One approach for simultaneously learning a model and 39 unknown external forcing is the "discrepancy modeling" frame-40 work (13-15). This fully Bayesian approach posits a model 41 of the same form as 1, where  $\delta(t)$  is the "discrepancy" and is 42 generally modeled as a Gaussian process. This and similar 43 frameworks have been applied in many different real-world 44 settings, including ecology (16), robotics (17), and control 45 (18). Gaussian processes are very powerful in that they can 46 model nearly any smooth function, but this contributes to a 47 major difficulty with this framework: identifiability (19, 20). 48 That is, unless you have many different data sets (21) or can 49 guess the functional form of the discrepancy (22), there is no 50 clear way to separate out what is the external signal and what 51 is the intrinsic dynamics. 52

We propose a new partially Bayesian framework called Sparse Residual Analysis (SRA)??? for learning sparsely active control signals purely from data simultaneous with an interpretable model of the intrinsic dynamics, allowing for accurate reconstructions both of the underlying autonomous system and the effects of the external signals. We do this by building the posterior distribution of a set of uncontrolled models,  $f(\mathbf{x})$ , either linear (DMD) or nonlinear (SINDy). Sampling from the posterior and comparing to data produces an initial guess for dynamics that are outside of the initial model structure, which forms a basis for approximating  $\delta(t)$ . We test our method on linear, nonlinear, and chaotic systems with external control signals, successfully learning the intrinsic simple system as well as the control signals.

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This paper proceeds as follows: Section II introduces the 67 background methods from statistical and machine learning; 68 Section III introduces our modified optimization problem and 69 practical subtleties with the algorithm; Section IV shows the 70 results of the method to decompose dynamics; and Section 71 V discusses future directions. The code for this framework is 72 freely available on GitHub in the programming language Julia, 73 heavily using advanced features from the DifferentialEquations 74 (23) and the Turing probabalistic programming packages (24). 75

## 2. Background Methods

Statistical Learning.As a complement to Machine Learning77methods which produce a black box prediction given data,78statistical learning methods seek to learn explicit and analyz-79able governing equations for a system, which can be linear or80nonlinear.81



Fig. 1. a) A simple example system: a bouncing ball. The intrinsic dynamics is the acceleration due to gravity, which is linear in the velocity-acceleration basis. The external spatially-dependent forcing is provided by the ground, and in this example there is an additional time-dependent forcing, e.g. a kick. b) The observed data in this simple case have obvious discontinuities, and the two types are easy to distinguish. c) The control signal provided by the ground, which is actually a function of space, and the external kick, which is purely a function of time.



Fig. 2. Beginning with data (in this case the Lorenz attractor with time-dependent external forcing), there are six steps to the model: 1. Fit a naive ODE. When integrated, this reconstruction will be very poor. 2. Find the posterior distribution of residuals of this naive ODE to numerically calculated derivatives. Note that this uses a collocation method, not integration. 3. Subsample the data, choosing the data points with small residual in the naive model. 4. Fit a "partial" model on the smaller sample of data. The control signals will not be captured, but the intrinsic dynamics may be. If they are not fit well, then looping back to step 2 will increase the quality of the subsample. 5. Using the residual of the final "partial" model, determine the control signals. 6. Fit the full control model, using control signals and data. This example is a chaotic system, so the individual trajectory will never be well reconstructed. Rather, the goal is to reconstruct the attractor.

<sup>82</sup> DMD and DMDc. DMD provides a linear model for data matrices

 $_{83}$  constructed using temporal snapshots of the state space,  $\mathbf{X} =$ 

<sup>84</sup>  $[\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_m]$  and  $\dot{\mathbf{X}} = [\dot{\mathbf{x}}_1 \ \dot{\mathbf{x}}_2 \ \dots \ \dot{\mathbf{x}}_m]$  where  $\mathbf{x}_j = \mathbf{x}(t_j)$ . <sup>85</sup> Specifically, it finds the best fit linear dynamical system

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$$\mathbf{X} = \mathbf{A}\mathbf{X}$$
 [2]

passing through the *m* snapshots of the statespace. There are a number of variants for computing A (1, 25? -29), with the *exact DMD* (25) simply constructing

$$\mathbf{A} = \dot{\mathbf{X}} \mathbf{X}^{\dagger}$$
 [3]

where † denotes the Moore-Penrose pseudo-inverse, which is
a least-squares fitting procedure. However, in practice due
to the size of matrix A in (3), the data is first projected
onto the dominant correlated modes via the singular value
decomposition before an eigen-decomposition is computed (30),
i.e. a low-rank approximation is first computed.

<sup>97</sup> DMDc (11) leverages the advantages of DMD and pro-<sup>98</sup> vides the additional innovation of disambiguating between the <sup>99</sup> underlying dynamics and the effects of a known actuation sig-<sup>100</sup> nal. For a control input matrix  $\mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \dots \ \mathbf{u}_{m-1}]$  where <sup>101</sup>  $\mathbf{u}_j = \mathbf{u}(t_j)$  is the actuation signal at time  $t_j$ , DMDc regresses <sup>102</sup> instead to the linear control system

$$\dot{\mathbf{X}} = \mathbf{A}\mathbf{X} + \mathbf{B}\mathbf{U}$$
[4]

The DMDc method regresses to find the best matrices **A** and **B** 104 in a least-squares sense given  $\mathbf{X}_1, \mathbf{X}_2$  and  $\mathbf{U}$ . Thus DMDc does 105 not require knowledge of the underlying governing equations, 106 only time snapshots of the state space and control input, 107 making it compelling for systems whose governing equations 108 are unknown. As with DMD, the DMDc algorithm capitalizes 109 on underlying low-dimensional structure in the data by using 110 the singular value decomposition to compute A and B in 111 practice. 112

113 SINDy and SINDYc. The SINDy algorithms have a parallel structure to the DMD equations above:

$$\dot{\mathbf{X}} = \mathbf{\Phi}(\mathbf{X})\mathbf{\Xi}$$
 [5]

And the formulation with control is similar:

$$\dot{\mathbf{X}} = \mathbf{\Phi}(\mathbf{X})\mathbf{\Xi} + \mathbf{B}\mathbf{U}$$
 [6]

where  $\Phi(\mathbf{X})$  is a library of nonlinear functions of the original data rows and  $\Xi$  is the sparse matrix of coefficients. Sparsity is enforced via an L1 norm or sequential least squares thresholding (12, 31), and significant parameters are determined via information theory metrics like AIC, as described in previous work (32).

Discrepancy modeling. Many inverse problems, that is learn-124 ing a model structure and parameter values from data, are 125 126 ill-posed TODO. There are multiple possible sources, and a major one is systematic discrepancy between the model and 127 data due to the data being produced by a process that does 128 not conform to the assumptions of the model. Seminal work 129 has demonstrated how direct modeling attempts can fail to 130 recover accurate dynamics, but they can be recovered if a 131 discrepancy term is added, as in Eq. 1 (13-15). This is done 132 by positing that  $\delta(t)$  can be modeled by a Gaussian Process, 133 i.e. a smooth function. 134

We take an opposite approach, positing sparsely active 135 or spike-like control signals. In this view, although the in-136 trinsic dynamics of the system could be modeled by Eqs. 5 137 or 2, a direct approach will not work because these external 138 perturbations are unknown. A key assumption is that these 139 external perturbations are sometimes weak or entirely absent, 140 allowing a subsampling procedure somewhat similar to (20). 141 Our approach then does not posit an explicit function form for 142  $\delta(t)$ , but instead treats this control function as the statistically 143 significant deviations between the intrinsic dynamics and the 144 data, where statistically significant refers to an explicit noise 145 model made possible due to the Bayesian framework. This 146 method is more fully explained in the next section and in 147 algorithm 1. 148

### 3. New method: SRA??

**Residual Analysis??.** Data generated from a linear process 150 with external shocks of the form in equation 4 can be fit using 151 an uncontrolled framework, for example via the least squares 152 method described in 3. In this case the regression matrix. 153 called  $\hat{\mathbf{A}}$ , may be very different from the true linear dynamics 154 A, because it is trying to account for the external input **BU**. 155 However, if we knew the dynamics, it would be very easy to 156 discover the control signals via rearranging equation 4: 157

$$\dot{\mathbf{X}} - \mathbf{A}\mathbf{X} = \mathbf{B}\mathbf{U}$$
 [7] 158

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Certainly, we do not know the true dynamics  $\mathbf{A}$ , but in many circumstances (TODO)  $\hat{\mathbf{A}}$  can be used to approximate this residual, and thus the control signals themselves. This extends to the nonlinear case, and if any parameters are known in advance these can be explicitly specified in this step. 160

**Probabilistic Programming.** It is possible to analyze a single 164 residual directly from equation 7. However, the residual of 165 any single model realization will be very sensitive to the exact 166 training data and noise. In some cases this sensitivity can be 167 mitigated, as shown in Fig. S3. A more statistically sound 168 alternative is to explore an ensemble of models, producing a 169 distribution of residuals. The presence of outliers beyond the 170 noise envelope is then very obvious, as the noise envelope is 171 explicitly modeled and fit. These outliers are then the initial 172 guess for the control signal, as shown in Fig. 2. 173

In addition, this Bayesian extension of the original SINDy algorithm automatically produces a posterior distribution for the model parameters as shown in Fig. 4.

**SRA??.** The full algorithm consists of a multi-step loop and 177 some preprocessing stages, as explained graphically in Fig. 178 2 and more generally in algorithm 1. Initially, the model 179 structure must be chosen, in this case either linear, as in Eq. 180 2 or nonlinear as is Eq. 5. This "naive" model is fit to the 181 derivative data. In some cases, particularly if the control 182 signals span multiple orders of magnitude, taking a random 183 intial subsampling can dramatically improve this naive model. 184

The next step is a loop that refines this initial model guess via modeling a well-selected subset of the data. This subset is the set of gradient points that is well reconstructed by the naive, uncontrolled model. "Well reconstructed" refers specifically to points whose errors are within a factor  $\lambda$  of the noise envelope. Note that these are reconstructions of the gradient itself via equation 1, and no integration of these Algorithm 1 Unsupervised Learning of Controlled Model

1: <b>I</b>	<b>procedure</b> LEARNCONTROLMODEL $(\mathbf{X}, \mathbf{\dot{X}})$	
2:	$\widehat{f}_0 := FitModelDistribution(\mathbf{\dot{X}})$	$\triangleright$ Eq. 2 or 5
3:	for $i \leftarrow 1, MaxIter$ do	
4:	$\mathbf{R}_i := \dot{\mathbf{X}} - \hat{f}_{i-1}(\dot{\mathbf{X}})$	⊳ E.g. eq. <b>7</b>
5:	$\dot{\mathbf{X}}_{i,sub} := Subsample(\dot{\mathbf{X}}, \mathbf{R}_i, \lambda)$	
6:	$\hat{f}_i := FitModelDistribution(\dot{\mathbf{X}}_{i,sub})$	
7:	$U_{final} := ProcessResidual(\mathbf{R}_{final})$	$\triangleright$ Sparsify
8:	$Model := Fit(\dot{\mathbf{X}}, \mathbf{X}, \hat{f}_{final}, U_{final})$	⊳ eq. 1

equations is performed. Last, once these "partial" models
have converged or after a maximum number of iterations, the
remaining residual between the final model and the data is
processed to form the final control signal.

There are three free hyperparameters or model choices 196 in this algorithm. First, the class of models must be cho-197 sen. In this paper, either linear (DMD) or sparse nonlinear 198 (SINDy) frameworks are chosen. Second, the threshold to use 199 for subsampling the points using the residual and the noise 200 envelope,  $\lambda$ . Third, the convergence criterion or maximum 201 number of iterations. All examples in this paper required a 202 single iteration. 203

#### 204 4. Results

Separation of linear dynamics. Fig 1 gives a very simple example for a dataset with linear intrinsic dynamics that can be analyzed using this method. The governing equations are simply the action of gravity:

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$$\dot{v} = a$$
  
 $\dot{a} = -g$ 

[8]

[10]

where the gravitational constant g = 9.81. However, the 210 two sources of external disturbance completely change the long-211 term behavior of the system, which would naturally simply 212 fall forever. In addition, these control signals only act on a 213 single variable directly: the acceleration. This means that a 214 naive linear model, one that does not account for control, will 215 successfully model the first term but not the second. The best 216 fit least-squares model to this data is: 217

$$\dot{v} = a$$
  
 $\dot{a} = -0.5v + 0.2a + 7.5$  [9

Extra terms appear, and "g" is incorrect. If this model 219 is integrated as in Fig. 1.?? the reconstruction is very bad, 220 however, this model is good enough to produce a good control 221 signal when doing point prediction of the derivative. The 222 residual between these point predictions and the data can be 223 processed as shown in Fig. 2 to produce the control signals 224 shown in Fig. 1.?? These control signals then produce a much 225 more accurate set of intrinsic dynamics, with  $g = -9.812 \pm$ 226 0.05??227

Learning nonlinear, chaotic dynamics. Many dynamical systems of interest are nonlinear, and many of these are chaotic.
One classic example, which was originally designed as a simplified model of atmospheric convection (33):

 $\dot{z} = xy - \beta z$ 

$$\dot{x} = \sigma(y-x)$$
  
32  $\dot{y} = x(
ho-z)-y$ 



**Fig. 3.** a) Voltage data from a spiking neuron model. The membrane recovery variable (u) is not shown, but is provided to the algorithm. b) The "control signal" in this case is then the fast nonlinearity, instead of a truly external input. The location is learned very accurately but because it is modeled as a true discontinuity in the equations, the exact amplitude of the derivative will depend sensitively on the sampling rate and the exact method used to numerically differentiate. c) However, if a varying input current is also applied, then this will show up as an additional control signal. d) The reset nonlinearity and and external voltage are learned as a single control signal. Importantly, the learned control signals are of very different orders of magnitude.



Fig. 4. Selected parameters are shown for the voltage (v) equation of Eq. 12. This algorithm successfully learns parameter values spanning four orders of magnitude with relatively small error. Note that even though there is no measurement error (white noise), some errors accumulate due to numerical differentiation.

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where  $\rho = 28$ ,  $\sigma = 10$ , and  $\beta = 8/3$ . This model can be 233 sparsely represented with a few analytic terms, and can be 234 recovered purely from data using the SINDy algorithm (31). 235 An unforced version of the attractor is shown in Fig. 2. 236

237 However, if there are external perturbations of unknown 238 magnitude, frequency, and input dimension, then the SINDy algorithm will not successfully recover the dynamics. For the 239 perturbed version of the attractor is shown in Fig. 2, the 240 SINDy algorithm with 2nd order library terms produces: 241

$$\dot{x} = -4.6x + 6.0y - 0.4z + 20.4$$
$$\dot{y} = 23.6x + 1.1y + 18.6 - 0.9xz \qquad [11]$$
$$\dot{z} = -2.7z + 1.0xy$$

In this dataset, control was only applied to the first two 243 variables (x and y), so the z equation is correct. Most of 244 the terms are similar but one has changed signs, and several 245 new erroneous terms have appeared. Integrating this naive 246 model, as shown for the x variable in Fig. 2, produces very 247 poor predictions. However, as Fig. 2 shows, as algorithm 1 248 is applied, the correct attractor and equations are recovered 249 along with the control signals. 250

Learning nonlinear, spiking dynamics. A model discrepancy 251 of the form in Eq. 1 may not be a true external input. In 252 particular, it could be a nonlinearity that happens very quickly 253 relative to data collection. One example is that of spiking 254 neurons, in the which the "reset" after a spike is defined as 255 256 instantaneous. A two dimensional model that can reproduce 257 spiking patterns from different classes of neurons (34) is:

$$\dot{v} = 0.04v^2 + 5v + 140 - u + I$$
$$\dot{u} = a(bv - u)$$
if v \ge 30 mV, then 
$$\begin{cases} v \leftarrow c \\ u \leftarrow u + d \end{cases}$$

[12]

Where I is the input current, the constants are chosen 259 as in the original paper to give v and t units of mV and 260 ms, respectively. u is a membrane recovery variable, and the 261 parameter values used here are those suggested: a = 0.02, 262 b = 0.2, c = -65, d = 2. The input current, I, is 40 for the 263 Constant Input neuron and is either 40 or 240 for the Variable 264 Input case in Fig. 3. 265

Discrepancy modeling as a field can have a problem of 266 identifiability (19), where the model for the discrepancy cannot 267 be distinguished from the core model. In this framework the 268 discrepancy can be any time series, with the assumption that it 269 is sparsely active, thus one identifiability problem can be that 270 271 of multiple control signals. As shown in 1, the control from the ground and the external forcing are learned as part of the single 272 time series that is input onto the second variable (acceleration). 273 A similar phenomenon happens with these spiking neurons, 274 where the "control signal" associated with resetting voltage 275 cannot be disentangled from modulation in external current 276 input, I, as demonstrated in Fig. 3. Nonetheless, the governing 277 equations are reconstructed very well, as shown in Fig. 4. 278

#### 5. Discussion 279

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Many data-driven modeling techniques posit that the dynam-280 ics present are autonomous in the chosen modeling framework. 281 However, this assumption may be violated in many ways, two 282

of which have been treated here: connections to the outside 283 environment, and very fast nonlinearities. Our unsupervised 284 modeling framework explicitly accounts for these external in-285 puts, and successfully models the underlying intrinsic dynamics 286 by pulling out the control signals or fast nonlinearities. 287

There are several assumptions that are necessary for good 288 numerical performance. For the examples studied in this paper 289 the intrinsic dynamics could be modeled by the imposed un-290 controlled model, and in particular for the nonlinear examples, 291 the true dynamics were sparse in the measured basis. This 292 issue of finding the correct basis is an active field of research in 293 this field TODO. A less well studied issue is that of the types 294 of control signals that can be successfully separated out from 295 "intrinsic" dynamics. This paper dealt with smooth intrinsic 296 dynamics and effectively discontinuous control signals, which 297 were thus separable because they could not be modeled with 298 the uncontrolled model. However, the other extreme is more 299 common in many fields. A popular controller in engineering 300 and potentially in many biological systems is a PID controller, 301 which uses terms proportional to simple functions of the state 302 in order to acheive control. This is by design continuous, and 303 in many cases the controlled system can be written as the 304 uncontrolled system with a change of parameters. This algo-305 rithm assumes that the structure and parameter values of the 306 intrinsic dynamics are unknown, and must be discovered along 307 with the control signal. However, if there is domain knowledge 308 of the intrinsic dynamics our algorithm may be extendable to 309 cases with smooth controllers, but this is outside the scope of 310 this work. 311

A separate limitation of this work is that a fully generative model is not produced. That is, extrapolation beyond 313 the training data can only be achieved for the uncontrolled, 314 intrinsic dynamics. Of course, if the control signal is truly ex-315 ternal, then extrapolation that requires such knowledge is not possible. However, if the "control signal" is actually a function of phase space, for example the ground in the bouncing ball example and the reset discontinuity in the neuron example, a generative model is possible but is not learned. For future work, it may be possible to separate out which portions of the learned control signal can be modeled as some function of the data, and which cannot.

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A universal difficulty is that of white noise, which is mag-324 nified in particular by two elements of the algorithm. First, 325 the need to take a numerical derivative, which is known to be 326 very sensitive to measurement noise. This is a well studied 327 problem (?), but there are no universal answers. Second, 328 because the residual of a naive model is an object of study, it is 329 vulnerable to large fluctuations. This second issue is mitigated 330 by a Bayesian framework for fitting the uncontrolled model. 331 Analyzing the posterior distribution of these residuals is a 332 much more robust procedure than analyzing a single residual, 333 but there are still no theoretical guarantees. Recent work on 334 simultaneous denoising and derivative calculations could be a 335 fruitful area of future work (35). 336

Our algorithm adds to the landscape of data-driven algorithms that derive symbolic governing equations and extends the range of applicability into new problem domains.

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