# "Deep" Dive in $b \rightarrow c$ Anomalies: Can we Automatize Model-Selection?



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## Inverse Problem

## **Forward Problem**

## Model 1, Model 2, ...

## **Inverse Problem**

Physical properties, Unknown parameters Measurements, Experimental Data

**Observables** 

## **Inverse Problem** (for Dummies like me)

9

## **Observation**

## Models





2.

## Inverse Problem (for Dummies like me)

## Reality

Image: Diet Wiegman



# Model Selection

- <u>Q</u>: Which is the best model to explain the data?
  - <u>Ans:</u> Whichever has minimum prediction error, i.e., optimum Bias and Variance.
    - Data → Statistical Inference → Model Selection
- <u>Cross-Validation</u>:
  - Powerful, reliable but computationally expensive
  - Draws on predictive error ⇒ can detect under and overfitting.
- <u>Caveats</u>:
  - 1. Error distribution to be known
  - 2. Small data-set  $\rightarrow$  becomes unstable

Beleites et al, ACA 760, 25 (2013), G. Varoquaux, (2017), arXiv:1706.07581 [q-bio.QM].

3. Small data-set + Comparable model size  $\Rightarrow$  No chance of doing anything!

## Alternatives?

- What to do for  $b \rightarrow c\tau v$  then?
  - 5  $C_W$ 's (Wilson Coefficients)  $\rightarrow C_{V_1}, C_{V_2}, C_{S_1}, C_{S_2}, C_T$
  - Each one complex  $\rightarrow$  total 10 parameters
  - 4 Observables: 9 Data-points (2018)
- We had used AIC<sub>C</sub> arXiv:1805.08222[EPJC 79, 268 (2019)]

Aritra is going to talk about these methods and their shortcomings in more detail... LOOCV, AIC<sub>c</sub> etc.

## Motivations

- No criterion tells the whole truth.
- All unstable for small sample sizes
- Depends on data at hand, whereas model predictions are available → have to redo everything for each change in data
- Depends on the MLE
   ⇒ no info. about span (uncertainty) of the datadist.
  - ⇒ Proclivity to select simpler models
- \*Bayesian Model Selection?\*

## (Ad Hoc) Bayesian Model Selection

- No 'true' model exists → data-distribution is 'true'
- Information lost to approximate a posterior P with a prior Q
  - This loss can be quantified by some '<u>divergence</u>' between P and Q
- Popular choice: Kullback–Leibler divergence (D<sub>KL</sub>)
  - Related to MLE, AIC, and cross-validation: more details in paper...
- 1. Find Bayesian parameter-space for all models
- 2. Find the predicted distributions of observables
- 3. Calculate  $D_{KL}$  for them
- 4. Lowest  $D_{KL} \rightarrow Best Model$

## $R(D) - R(D^*)$ Status (2019)



## $R(D) - R(D^*)$ Status (2019)

Observables		Measurement
$\mathcal{R}_D[6]$	)	0.340(27)(13)
$\mathcal{R}_{D^*}$ [6]	4-obs_data-set	0.295(11)(8)
$P_{\tau}(D^*)$ [40]		$-0.38(51)( \begin{array}{c} +0.21\\ -0.16 \end{array})$
$F_L^{D^*}$ [35]	New Lattice: arXiv:2007.06956	0.60(8)(4)
$\mathcal{R}_{J/\psi}$ [12]	SM: 0.2601 ±0.0036	0.71(17)(18)

## Complexity of Inverse Problem



## Complexity of Inverse Problem





# Proposal



## Probable Inverse Functions



## Probable Inverse Functions



## Probable Inverse Functions



## Neural Network: SNN

- Self-Normalizing Neural-networks: proposed in 2017 [Klambauer et al, arXiv:1706.02515]
- Solves <u>gradient-vanishing/exploding</u> problem of traditional Fully-Connected-Networks
- Enables 'deep' networks
   ⇒ Performance ≥ shallow algorithms
- Special activation function: SELU
- Variation remains normalized over the whole network.
- (Modified) Dropout layers possible
   ⇒ Enables Regularization, \*Bayesian Networks\*

## Neural Network: SNN

Classifier	Accuracy
ensemble-SNN	89.08%
Random Forest	82.70%
Decision Tree	78.27%
Nearest Neighbors	74.22%
Gradient Boosted Trees	74.10%
Support Vector Machine	63.82%
Markov Process	50.76%
Naive Bayes	46.64%
Logistic Regression	29.80%



## *SNN* → *Ensemble SNN*



	Input	vector (size: 4)
1	NetChain (3 nodes)	vector (size: 50)
2	NetChain (3 nodes)	vector (size: 50)
3	NetChain (3 nodes)	vector (size: 50)
4	NetChain (3 nodes)	vector (size: 50)
5	NetChain (3 nodes)	vector (size: 50)
6	NetChain (3 nodes)	vector (size: 50)
7	NetChain (3 nodes)	vector (size: 50)
8	LinearLayer	vector (size: 20)
9	SoftmaxLayer	vector (size: 20)
	Output	vector (size: 20)

1: NetChain

#### Input

- LinearLayer
- ScaledExponentialLinearUnit[x]
- 3 DropoutLayer Output

- vector (size: 4)
- vector (size: 50)
- vector (size: 50)
- vector (size: 50)
- vector (size: 50)

## $SNN \rightarrow Ensemble SNN$



## Classification Results

Data-Set	Models	Parameters	Aggregate	$D_{KL}$	SNN-Central	$\Delta AIC_c$	$w^{\Delta AIC_c}$
	(SNN-Aggregate)		Prob. (%)	Serial	Serial	Serial	(%)
	12	$Re(C_{V_2}), Re(C_T)$	38.48	2	1	18	0.07
	15	$Re(C_{S_2}), Re(C_T)$	<b>26.30</b>	3	5	6	0.32
	13	$Re(C_{S_1}), Re(C_{S_2})$	11.53	9	7	9	0.29
	14	$Re(C_{S_1}), Re(C_T)$	8.04	1	15	17	0.11
4-Obs.	8	$Re(C_{V_1}), Re(C_{S_2})$	5.01	18	3	7	0.32
	10	$Re(C_{V_2}), Re(C_{S_1})$	2.80	6	<b>2</b>	11	0.16
	6	$Re(C_{V_1}), Re(C_{V_2})$	2.19	14	9	12	0.12
	11	$Re(C_{V_2}), Re(C_{S_2})$	1.74	4	4	8	0.32
	19	$C_{S_2}$	1.18	17	6	10	0.29
3. <del>3</del>	12	$Re(C_{V_2}), Re(C_T)$	42.62	1	2	17	0.69
	13	$Re(C_{S_1}), Re(C_{S_2})$	15.71	19	6	7	3.19
	15	$Re(C_{S_2}), Re(C_T)$	8.56	4	10	4	3.37
	6	$Re(C_{V_1}), Re(C_{V_2})$	6.7	16	12	11	1.33
5-Obs.	8	$Re(C_{V_1}), Re(C_{S_2})$	6.54	18	4	5	<b>3.31</b>
	14	$Re(C_{S_1}), Re(C_T)$	6.09	2	7	15	1.14
	7	$Re(C_{V_1}), Re(C_{S_1})$	4.63	8	11	12	1.29
	11	$Re(C_{V_2}), Re(C_{S_2})$	3.7	3	3	6	3.3
	10	$Re(C_{V_2}), Re(C_{S_1})$	2.66	6	1	9	1.67
	17	$C_{V_2}$	1.45	15	9	10	1.33

## Predictions: Test Model - 15



## Observables:



## Predictions + Classification

Dataset	Model Index	1	$O_{KL}$
		(Net)	(Bayes)
	15	3.75	31.78
	14	10.43	$1.15 \times 10^5$
4-Obs.	10	14.53	$1.21 \times 10^{6}$
	12	18.20	$6.53 \times 10^{4}$
	11	29.67	$5.49 \times 10^5$
	12	95.60	$6.29 \times 10^{6}$
	15	1146.50	$1.92 \times 10^6$
5-Obs.	14	1631.02	$9.60 \times 10^{7}$
	10	3232.05	$5.20 \times 10^{6}$
	11	3905.8	$2.41 \times 10^6$

## Predictions + Classification

Dataset	Model Inde	Model Index		(%)
		$\sigma$	$R^2$	MSE
	15	1.80	99.93	0.03
	14	2.03	99.91	0.04
4-Obs.	10	3.08	99.84	0.10
	12	1.30	99.93	0.02
x	11	2.34	99.91	0.05
	12	1.58	99.90	0.02
	15	2.19	99.89	0.05
5-Obs.	14	2.33	99.88	0.05
	10	3.28	99.82	0.11
	11	2.97	99.86	0.09

## Future: This mode

- There are other, unmeasured observables:
  - 1.  $B \rightarrow D^{(*)}\tau\nu$ :  $\mathcal{A}_{FB}^{(*)}$ ,  $P_{\tau}(D)$ 2.  $\Lambda_h \to \Lambda_c \tau \nu_\tau : \mathcal{R}^{\ell}_{\Lambda}, \mathcal{A}^{\Lambda}_{FB}$
  - \*13 in Total\* 3.  $B_c \rightarrow J/\Psi \tau \nu_{\tau} : \mathcal{A}_{FR}^{J/\Psi}, P_{\tau}(J/\Psi), F_L(J/\Psi)$
  - 4. And updates on all present ones...
- We trained another full set of classifier and predictor SNNs for all 'models'... because we can!
  - Their tests will only happen when data appears...
- In the mean time, let's see what happens to the predictions with future luminosities: (central values kept same, uncertainties decreased)

#### Future: This mode 0.4Model: 12 Model: 14 0.2 0.30.1 0.2 $Re(C_T)$ $Re(C_T)$ 0. 0.0 0.0-0.1-0.10.05 Model: 15 -0.2 -1.0-0.50.0 0.2 0.4 0.6 0.8 1.1 Re(Cy.) Re(Cs.) 0.00 -0.05Re(C<sub>7</sub>) 01'0--0.15 -0.20-0.25-0.50.0 0.5 -2.0 -1.5 -1.0Re(Cs.)

## Future: Other observables?

- Global  $\mathbf{b} \rightarrow \mathbf{s} \ell \ell$  ?
  - 9  $C_W$ 's (Wilson Coefficients)  $\rightarrow C_7, \Delta C_9, C_9, \Delta C_{10}, C_{10}, C_S, C_S, C_P, C_P$
  - If all are Complex  $\rightarrow$  1022 combinations
  - > 200 obs. ⇒ Cross Validation, Bayesian Model Selection possible
  - Enough data for full classification and precise prediction: Preliminary tests: > 99% accuracy
  - Varying network structure, calculating prediction error much more important.
- Electroweak Data + Higgs Decays → SMEFT model independent predictions?
- Why stop there? Compare classes of BSM models...



Play around with our trained networks
 → classifiers, predictors and Bayesian Results...

https://github.com/FlavorIITG/MLResourcesForSemileptonic-b2c

• An interactive web applet will come soon ...

# FIGNES

### Back-Up: Error-Rate Plots





60



0.4

0.4

Best Round

Rounds



Best Round

Rounds

## **Other Properties**

10

Training Info.	Details
Batches/Round	170
Batch Size	10000
Best Valid. Round	20
${\rm Final}\ell$	0.0009998
Initial $\ell$	0.001
Avg. Batches/Second	81.65
Final Round Loss	0.406
Final Round Error	14.48%
Total Batches	7820
Total Rounds	46
Validation Loss	0.51
Validation Error-Rate	21%

## **Other Properties**

Measure	4  Obs.	5 Obs.	13 Obs.
Accuracy	85.88%	88.67%	89.68%
Cohen's $\kappa$	85.14%	88.08%	89.42%
Error	14.12%	11.33%	10.32%
Geometric Mean Prob.	69.54%	71.97%	71.75%
Mean Cross-Entropy	0.363	0.329	0.332
Mean Decision Utility	85.88%	88.67%	89.68%
Perplexity	1.44	1.39	1.39
Scott's $\pi$	85.13%	88.07%	89.42%

## **Confusion Matrices**







## Back-Up: $b \rightarrow c$

$$\begin{aligned} \mathcal{H}_{eff} &= \frac{4G_F}{\sqrt{2}} V_{cb} \Big[ (\delta_{\ell\tau} + C_{V_1}^\ell) \mathcal{O}_{V_1}^\ell + C_{V_2}^\ell \mathcal{O}_{V_2}^\ell \\ &+ C_{S_1}^\ell \mathcal{O}_{S_1}^\ell + C_{S_2}^\ell \mathcal{O}_{S_2}^\ell + C_T^\ell \mathcal{O}_T^\ell \Big], \end{aligned}$$

$$\mathcal{O}_{V_1}^{\ell} = (\bar{c}_L \gamma^{\mu} b_L) (\bar{\tau}_L \gamma_{\mu} \nu_{\ell L}),$$
  

$$\mathcal{O}_{V_2}^{\ell} = (\bar{c}_R \gamma^{\mu} b_R) (\bar{\tau}_L \gamma_{\mu} \nu_{\ell L}),$$
  

$$\mathcal{O}_{S_1}^{\ell} = (\bar{c}_L b_R) (\bar{\tau}_R \nu_{\ell L}),$$
  

$$\mathcal{O}_{S_2}^{\ell} = (\bar{c}_R b_L) (\bar{\tau}_R \nu_{\ell L}),$$
  

$$\mathcal{O}_T^{\ell} = (\bar{c}_R \sigma^{\mu\nu} b_L) (\bar{\tau}_R \sigma_{\mu\nu} \nu_{\ell L}),$$

Wilson coefficients  $\rightarrow C_W^{\ell}$ 

Models

Index	Parameters	Index	Parameters
1(1)	$\operatorname{Re}(C_{V_1})$	16	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1})$
2(2)	$\operatorname{Re}(C_{V_2})$	17	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_2})$
3(3)	$\operatorname{Re}(C_{S_1})$	18	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2}), \operatorname{Re}(C_T)$
4(4)	$\operatorname{Re}(C_{S_2})$	19	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2})$
5(5)	$\operatorname{Re}(C_T)$	20	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_T)$
6(6)	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2})$	21	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$
7(7)	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{S_1})$	22	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2})$
8(8)	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{S_2})$	23	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_T)$
9(9)	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_T)$	24	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$
10(10)	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1})$	25	$\operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$
11(11)	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_2})$	26	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2})$
12(12)	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_T)$	27	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_T)$
13(13)	$\operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2})$	28	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$
14(14)	$\operatorname{Re}(C_{S_1}), \operatorname{Re}(C_T)$	<b>29</b>	$\operatorname{Re}(C_{V_1}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$
15(15)	$\operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$	30	$\operatorname{Re}(C_{V_2}), \operatorname{Re}(C_{S_1}), \operatorname{Re}(C_{S_2}), \operatorname{Re}(C_T)$

## Models

Index	Parameters
31(16)	$C_{V_1}$
32(17)	$C_{V_2}$
33(18)	$C_{S_1}$
34(19)	$C_{S_2}$
35(20)	$C_T$
36	$C_{V_1}, C_{V_2}$
37	$C_{V_1}, C_{S_1}$
38	$C_{V_1}, C_{S_2}$
39	$C_{V_1}, C_T$
40	$C_{V_2}, C_{S_1}$
41	$C_{V_2}, C_{S_2}$
42	$C_{V_2}, C_T$
43	$C_{S_1}, C_{S_2}$
44	$C_{S_1}, C_T$
45	$C_{S_2}, C_T$