Knowing when to Quit:

Why do we waste so much time trying to get models out of bad data?

Barry M. Wise and Jeremy M. Shaver
Eigenvector Research, Inc.

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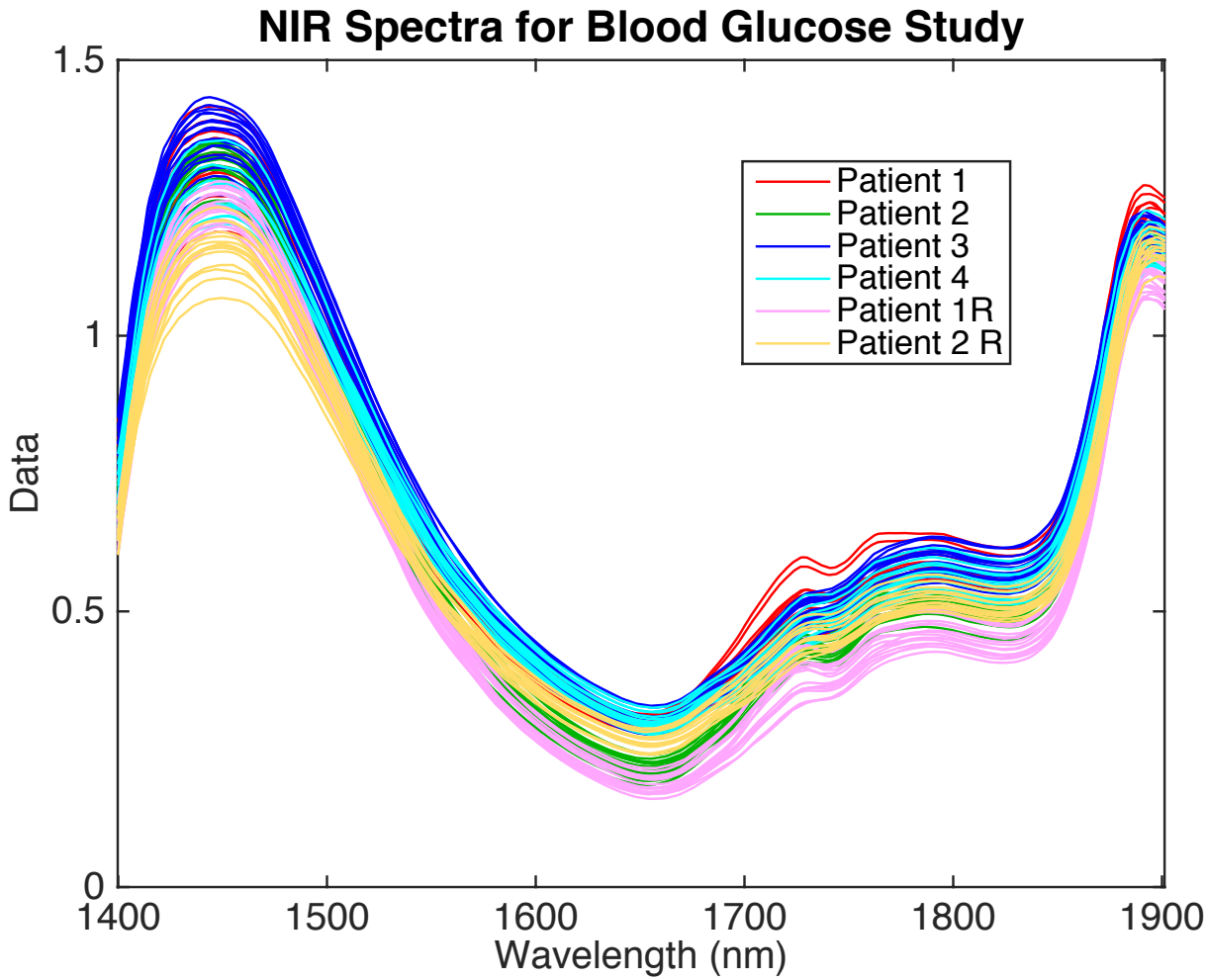
Outline

- The Problem
- An example
- Conclusion
- Discussion

The Problem

- Lots of bad data out there!
- Engineers and scientists developing methods based on more complex signals
  - Using spectroscopy on everything!
- Problems complicated by low signal-to-noise and/or low signal-to-clutter
  - Blood glucose
- May not be possible to get a reasonable model in some of these situations

Example Data Set
Blood glucose by NIR (again!)



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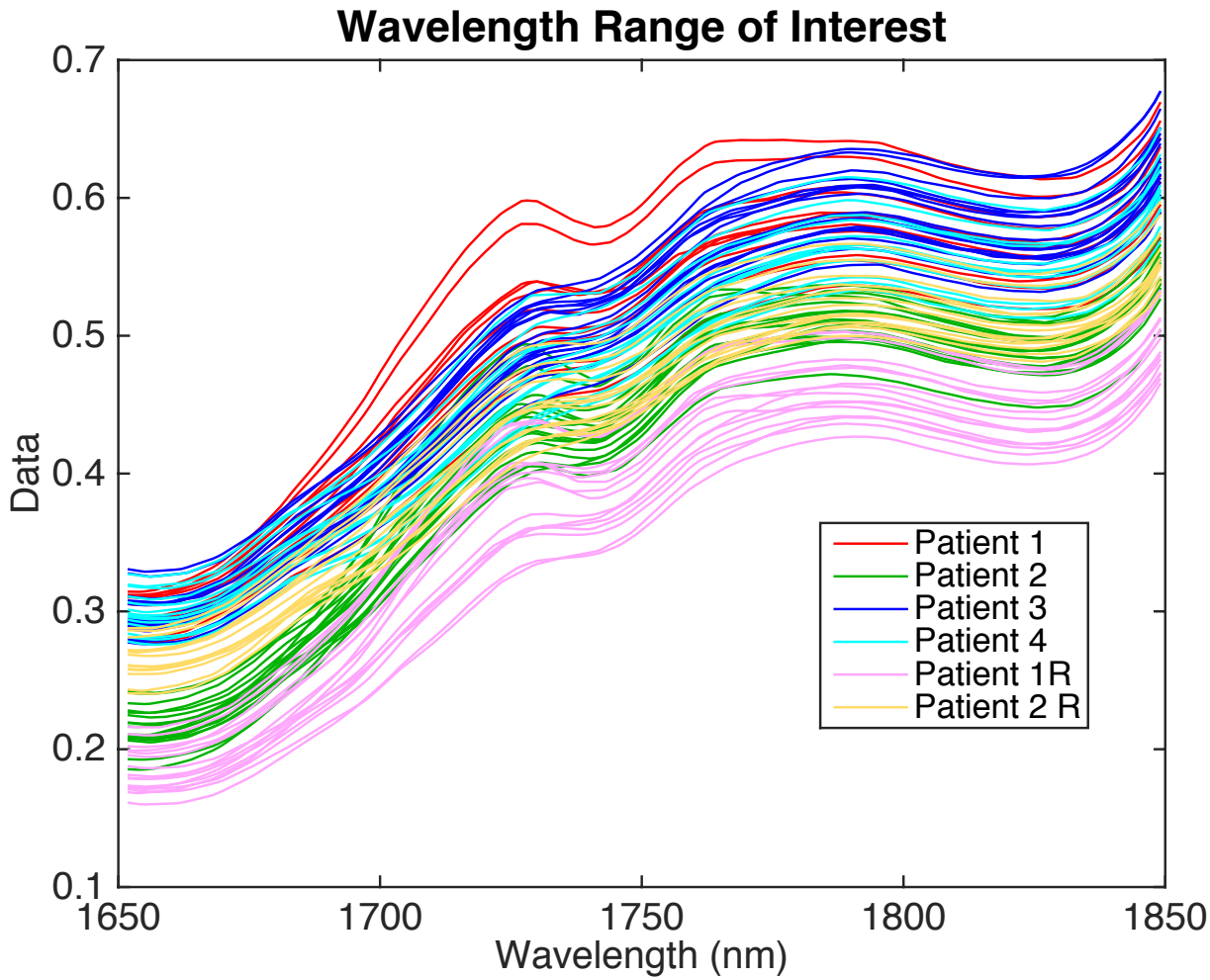
Region of Interest



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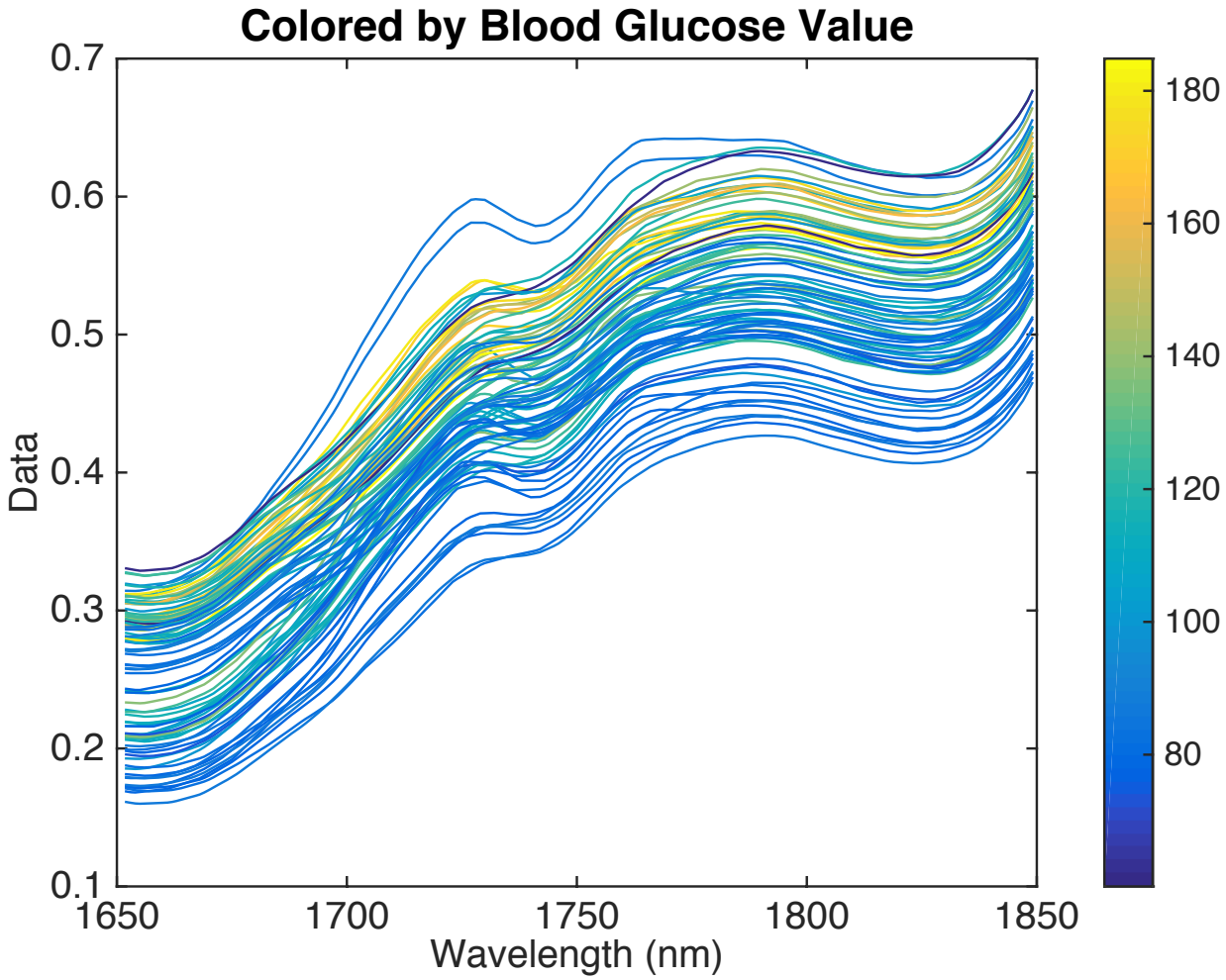
What to try

- Basic “plain vanilla” models
- Look at preprocessed data and color-by
- Nearly exhaustive search—Model Optimizer
  - Try to stick with “reasonable” preprocessing
- Interrogate best models
  - Over-fit?
  - Any reason model be over-optimistic?
  - Squint test

No Obvious Trend



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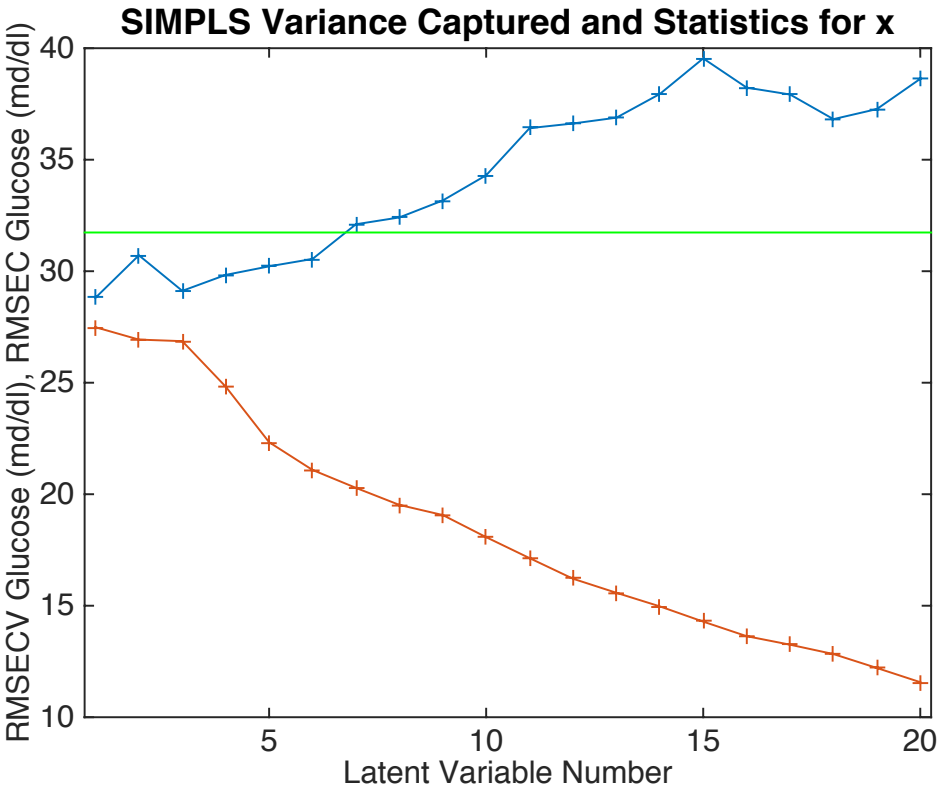
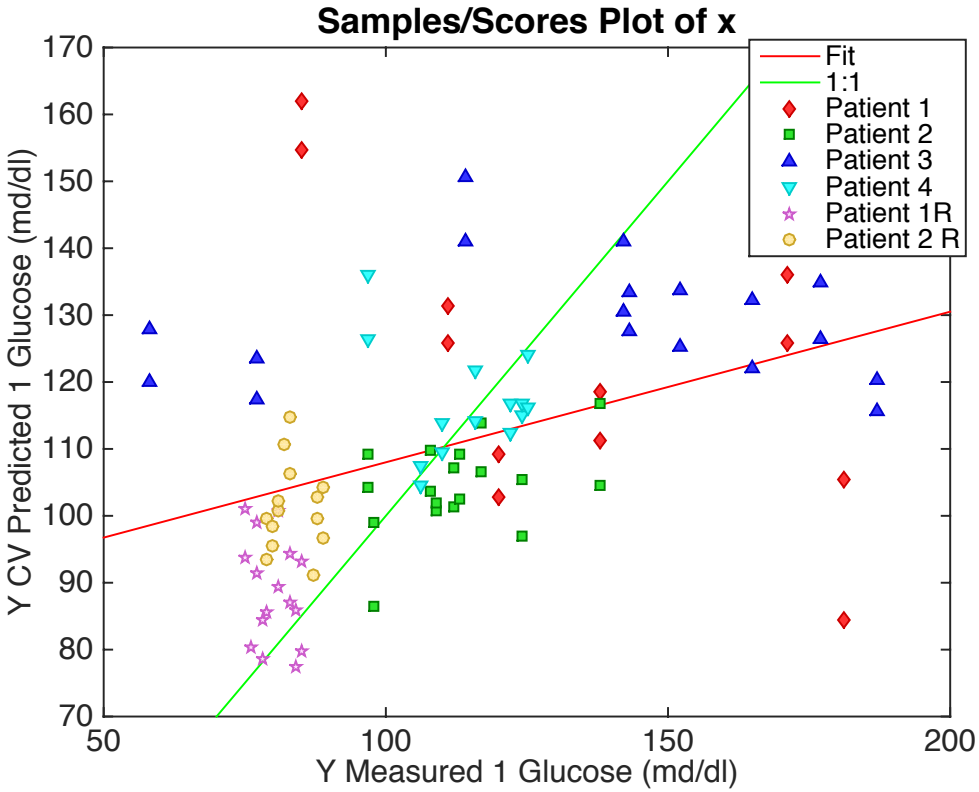
Initial Model





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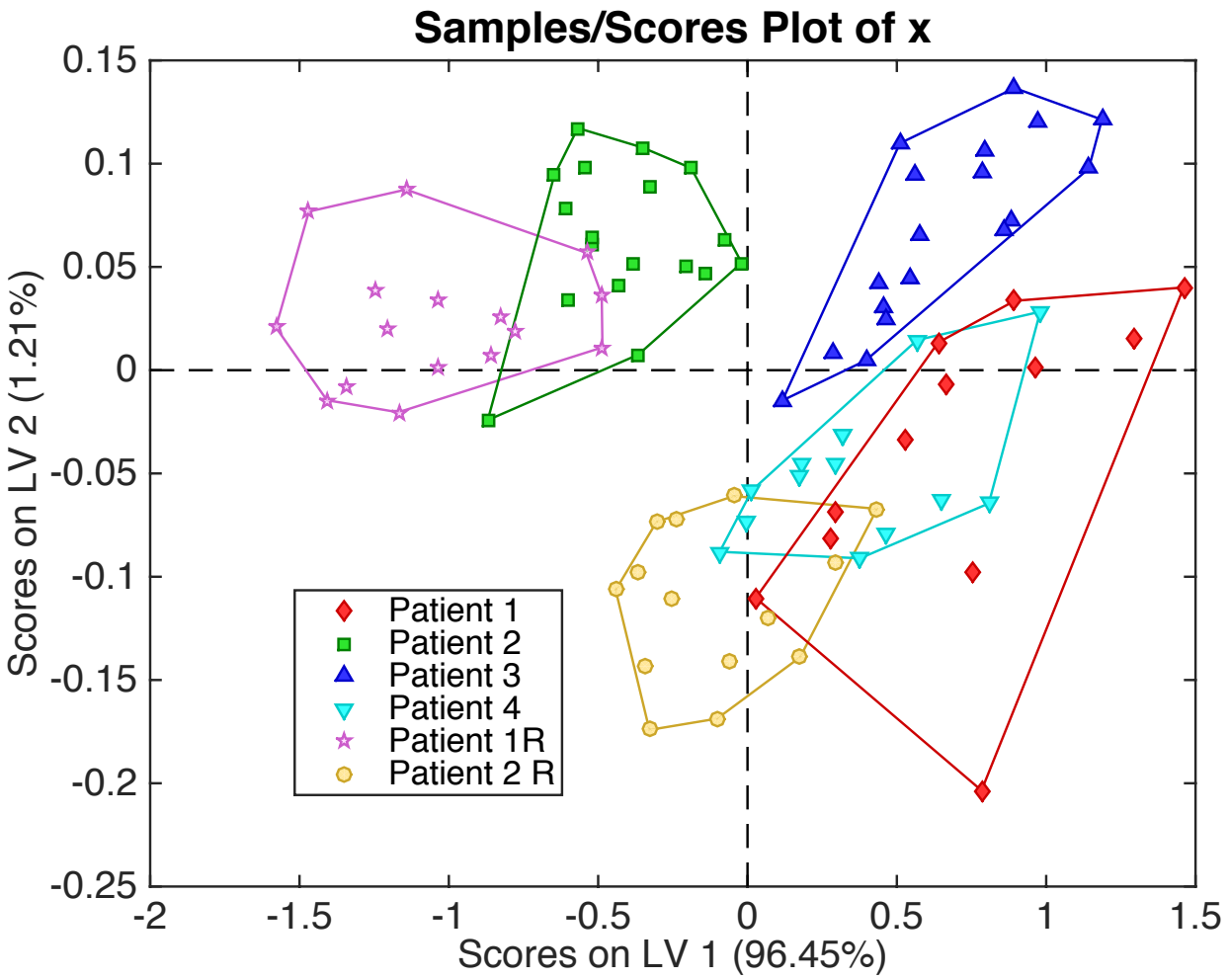
Scores from MC Model



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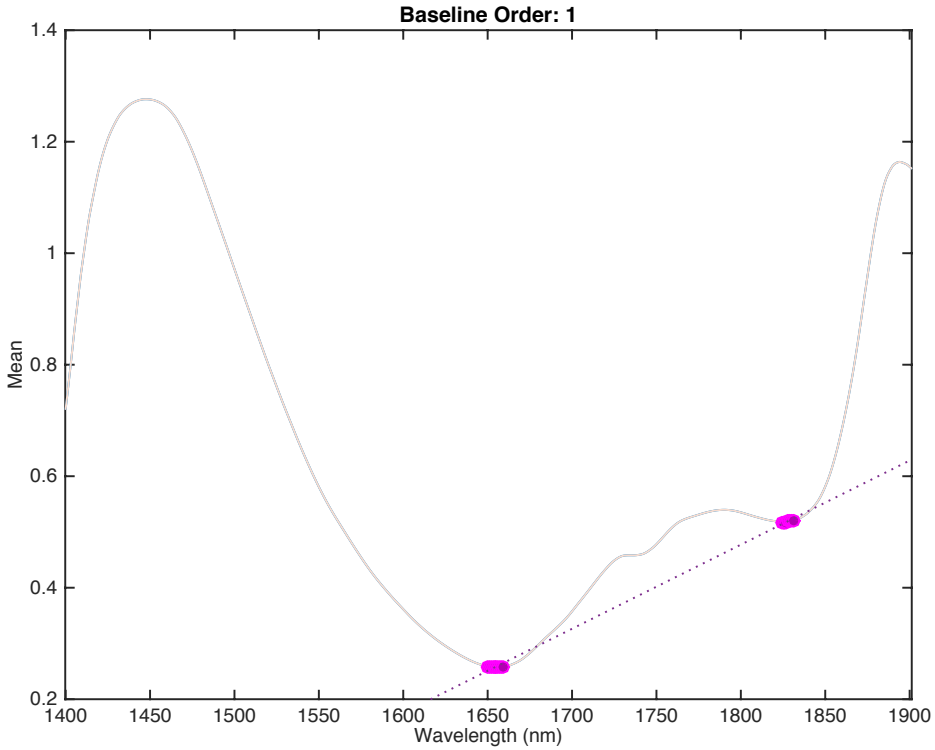
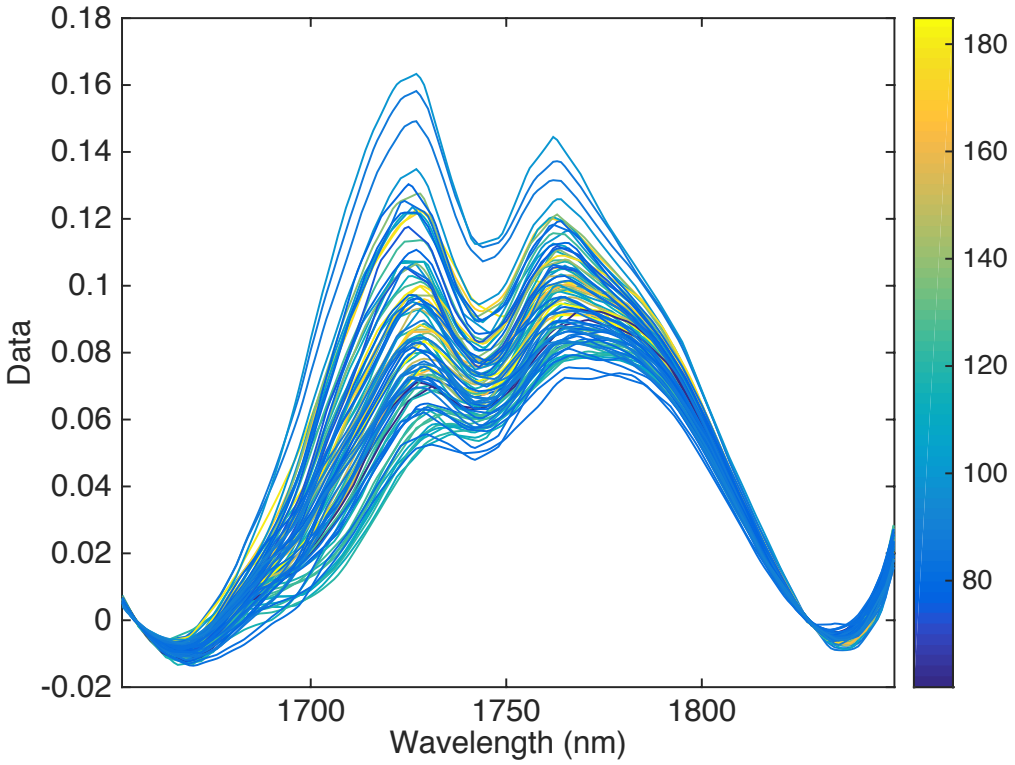
Try Different Preprocessing





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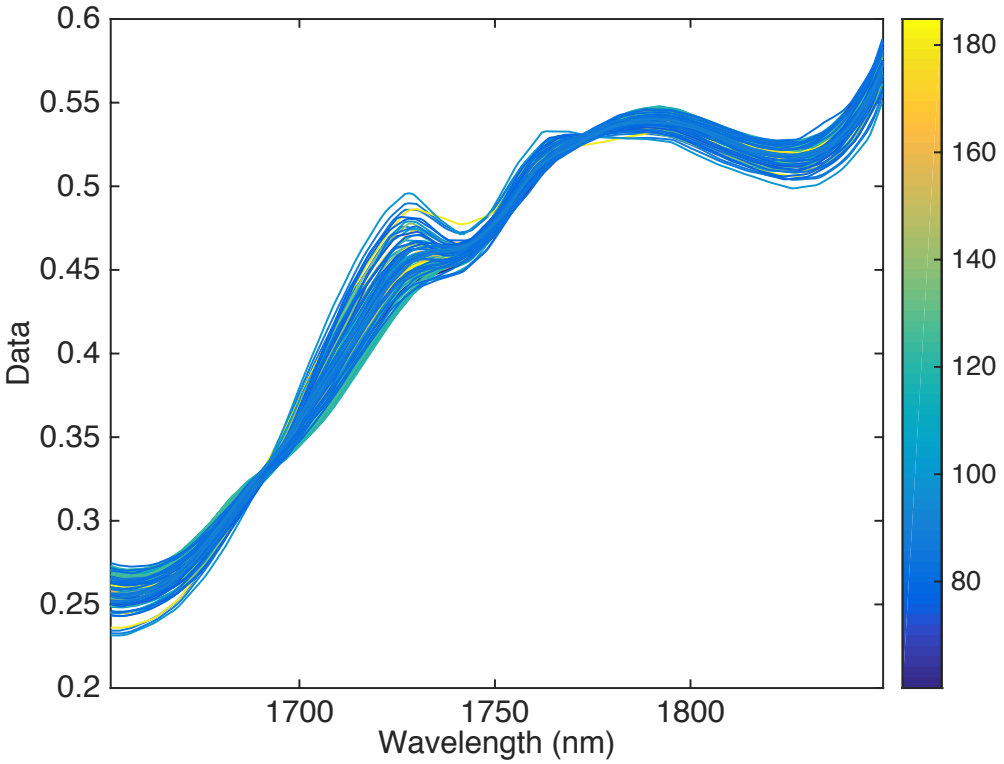
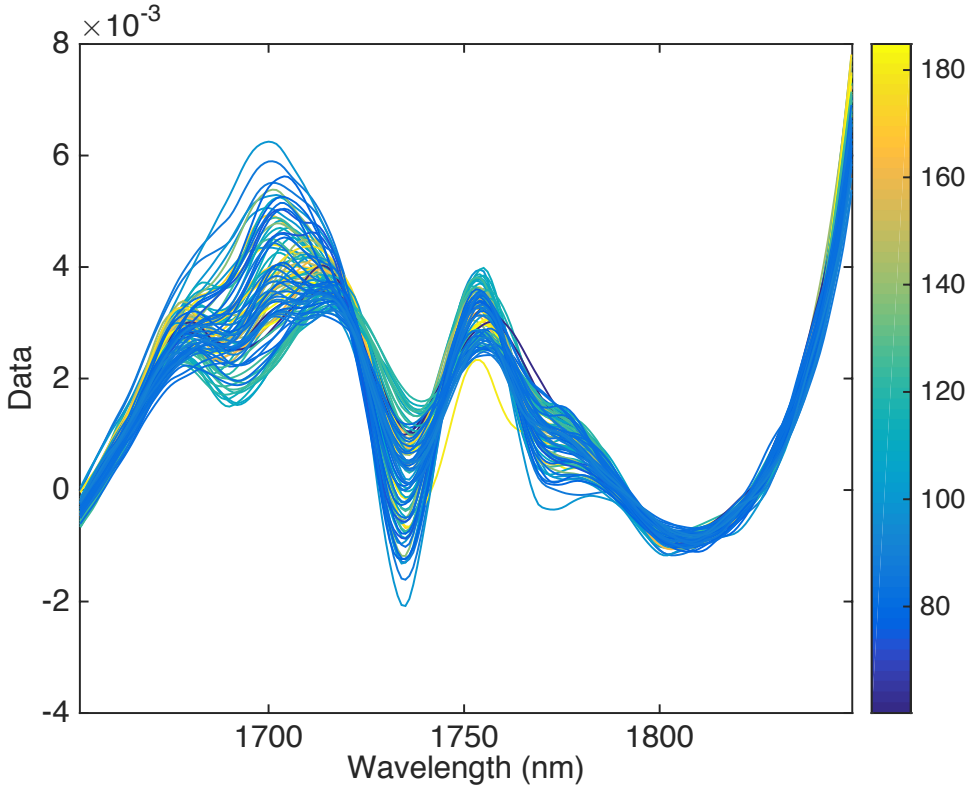
Other Preprocessing





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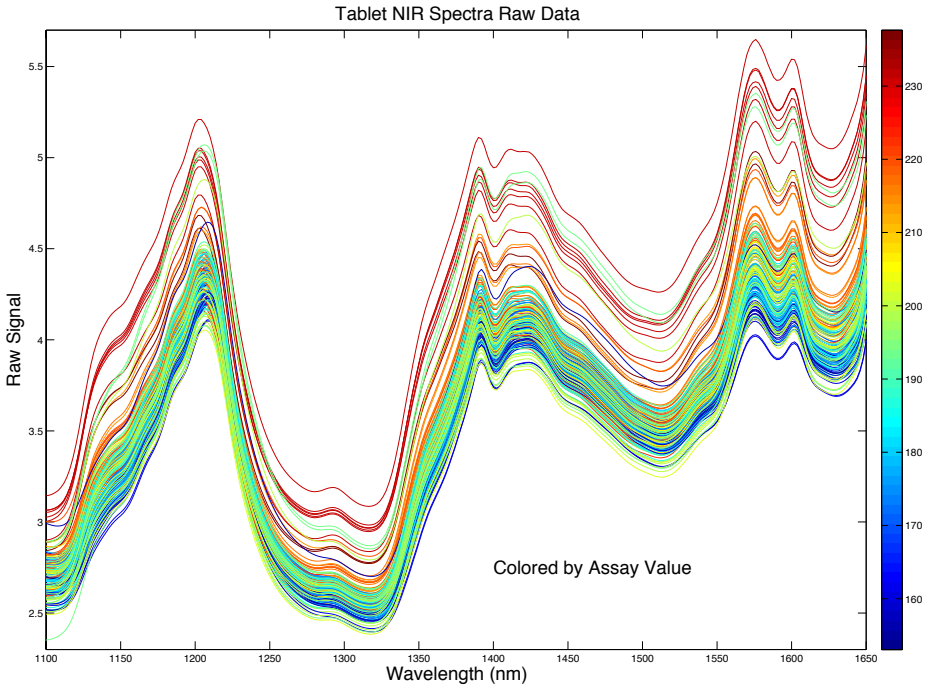
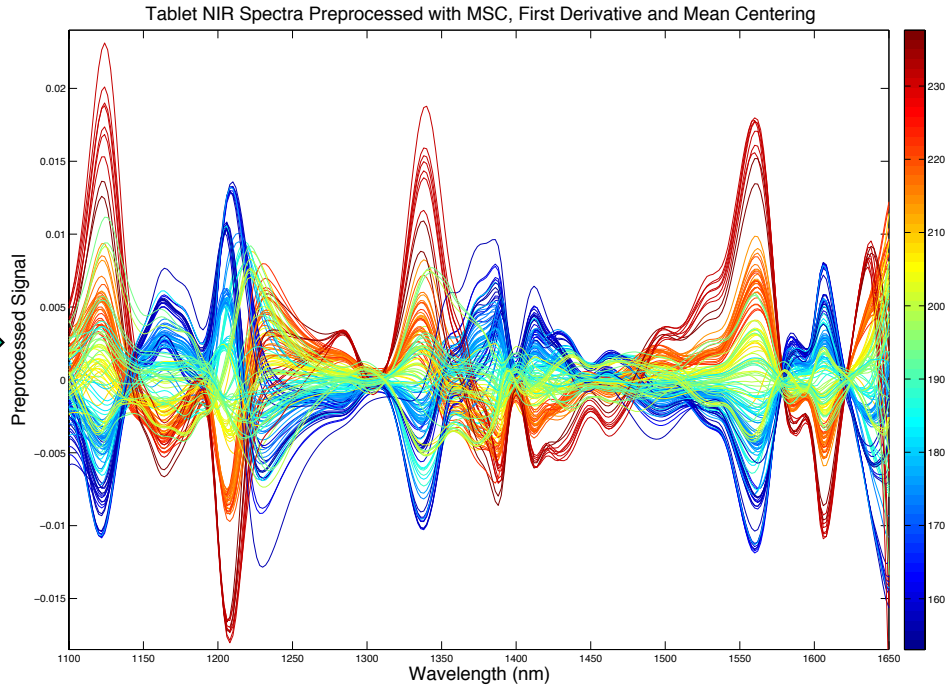
When Preprocessing Works!





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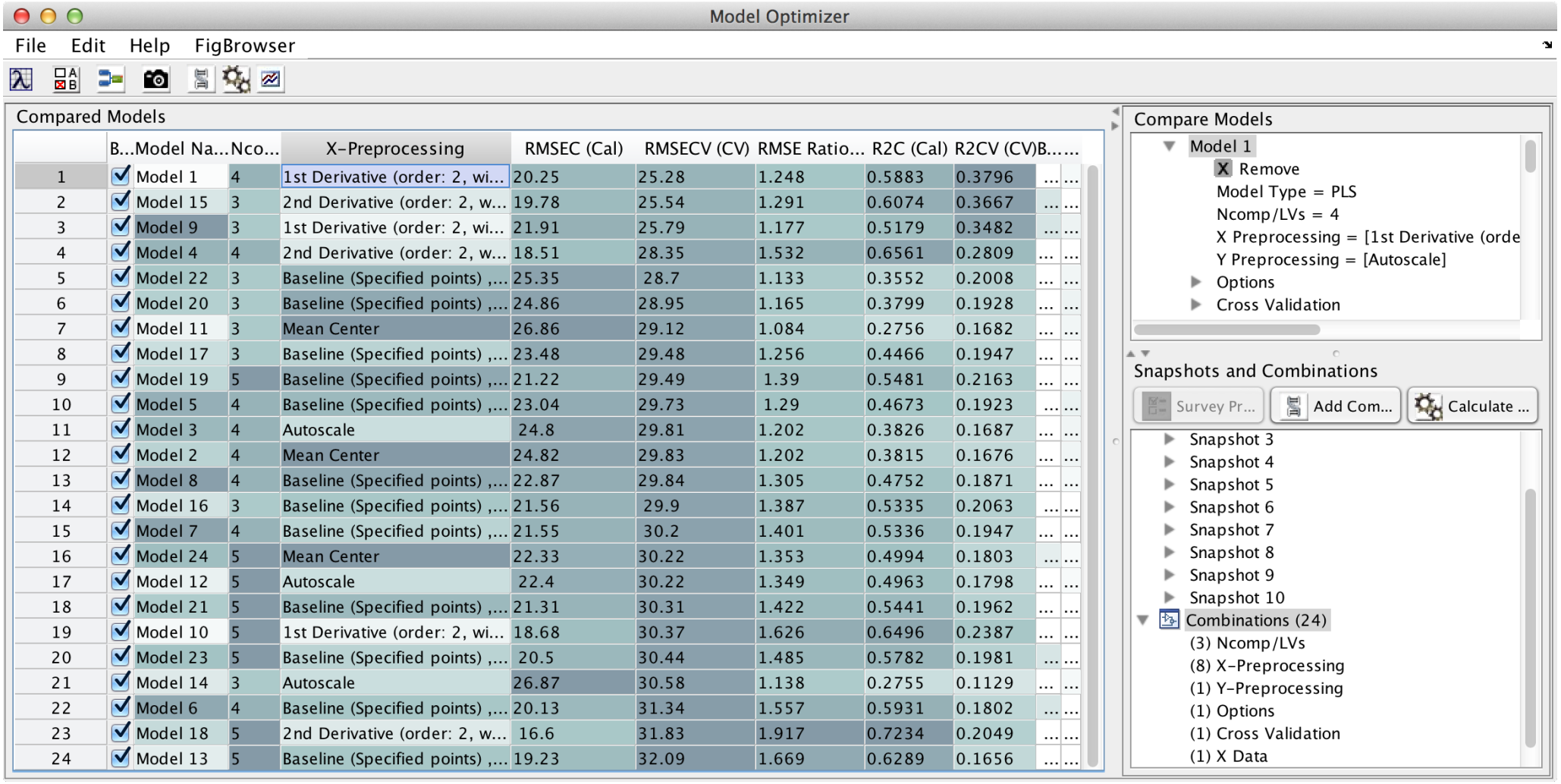
Model Optimizer



	B...	Model Na...	Nco...	X-Preprocessing	RMSEC (Cal)	RMSECV (CV)	RMSE Ratio...	R2C (Cal)	R2CV (CV)	B.....
1	☑	Model 1	4	1st Derivative (order: 2, wi...	20.25	25.28	1.248	0.5883	0.3796	... ...
2	☑	Model 15	3	2nd Derivative (order: 2, w...	19.78	25.54	1.291	0.6074	0.3667	... ...
3	☑	Model 9	3	1st Derivative (order: 2, wi...	21.91	25.79	1.177	0.5179	0.3482	... ...
4	☑	Model 4	4	2nd Derivative (order: 2, w...	18.51	28.35	1.532	0.6561	0.2809	... ...
5	☑	Model 22	3	Baseline (Specified points) ,...	25.35	28.7	1.133	0.3552	0.2008	... ...
6	☑	Model 20	3	Baseline (Specified points) ,...	24.86	28.95	1.165	0.3799	0.1928	... ...
7	☑	Model 11	3	Mean Center	26.86	29.12	1.084	0.2756	0.1682	... ...
8	☑	Model 17	3	Baseline (Specified points) ,...	23.48	29.48	1.256	0.4466	0.1947	... ...
9	☑	Model 19	5	Baseline (Specified points) ,...	21.22	29.49	1.39	0.5481	0.2163	... ...
10	☑	Model 5	4	Baseline (Specified points) ,...	23.04	29.73	1.29	0.4673	0.1923	... ...
11	☑	Model 3	4	Autoscale	24.8	29.81	1.202	0.3826	0.1687	... ...
12	☑	Model 2	4	Mean Center	24.82	29.83	1.202	0.3815	0.1676	... ...
13	☑	Model 8	4	Baseline (Specified points) ,...	22.87	29.84	1.305	0.4752	0.1871	... ...
14	☑	Model 16	3	Baseline (Specified points) ,...	21.56	29.9	1.387	0.5335	0.2063	... ...
15	☑	Model 7	4	Baseline (Specified points) ,...	21.55	30.2	1.401	0.5336	0.1947	... ...
16	☑	Model 24	5	Mean Center	22.33	30.22	1.353	0.4994	0.1803	... ...
17	☑	Model 12	5	Autoscale	22.4	30.22	1.349	0.4963	0.1798	... ...
18	☑	Model 21	5	Baseline (Specified points) ,...	21.31	30.31	1.422	0.5441	0.1962	... ...
19	☑	Model 10	5	1st Derivative (order: 2, wi...	18.68	30.37	1.626	0.6496	0.2387	... ...
20	☑	Model 23	5	Baseline (Specified points) ,...	20.5	30.44	1.485	0.5782	0.1981	... ...
21	☑	Model 14	3	Autoscale	26.87	30.58	1.138	0.2755	0.1129	... ...
22	☑	Model 6	4	Baseline (Specified points) ,...	20.13	31.34	1.557	0.5931	0.1802	... ...
23	☑	Model 18	5	2nd Derivative (order: 2, w...	16.6	31.83	1.917	0.7234	0.2049	... ...
24	☑	Model 13	5	Baseline (Specified points) ,...	19.23	32.09	1.669	0.6289	0.1656	... ...

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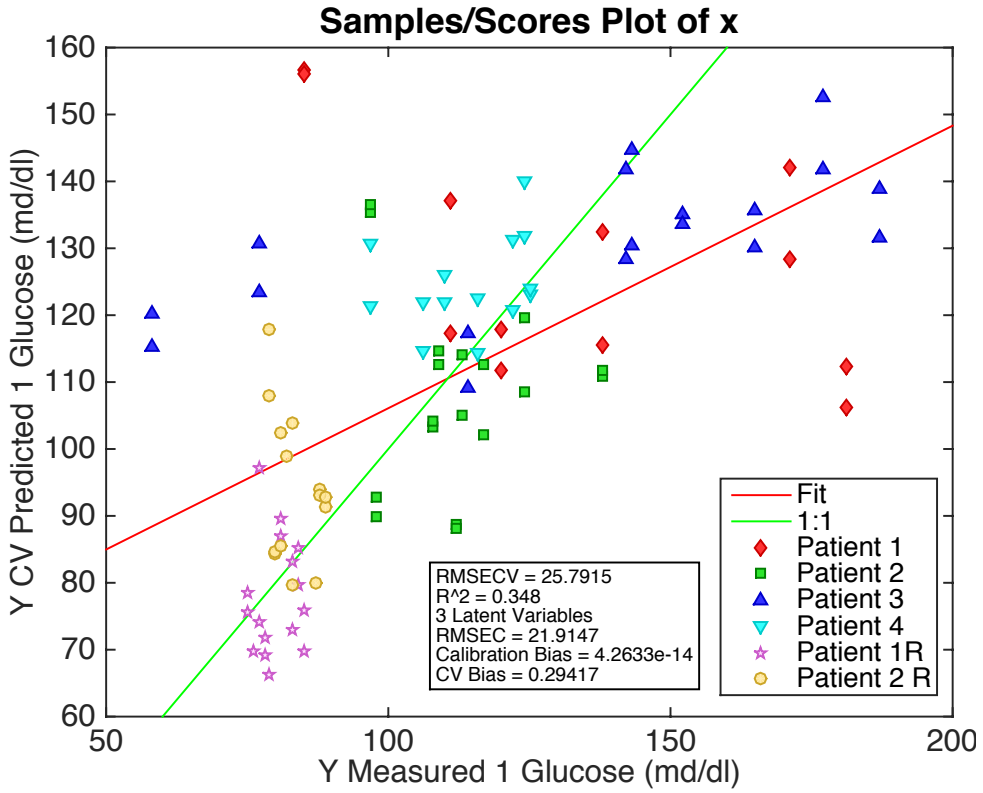
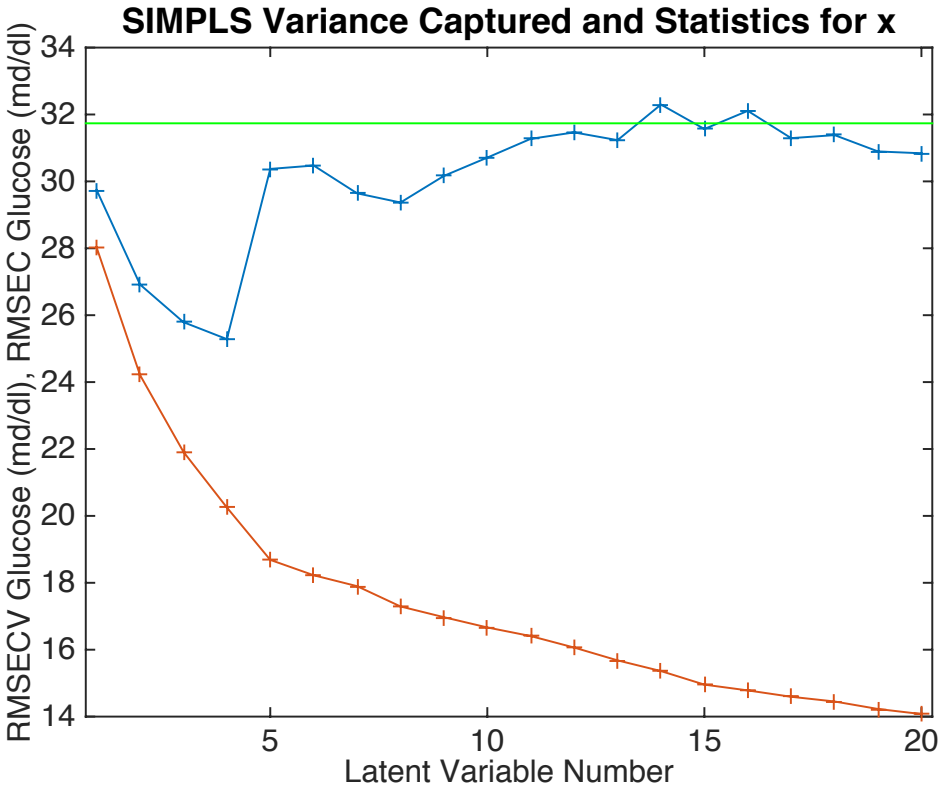
Best Model Replicate CV





Cross-validation by replicate (46 splits)

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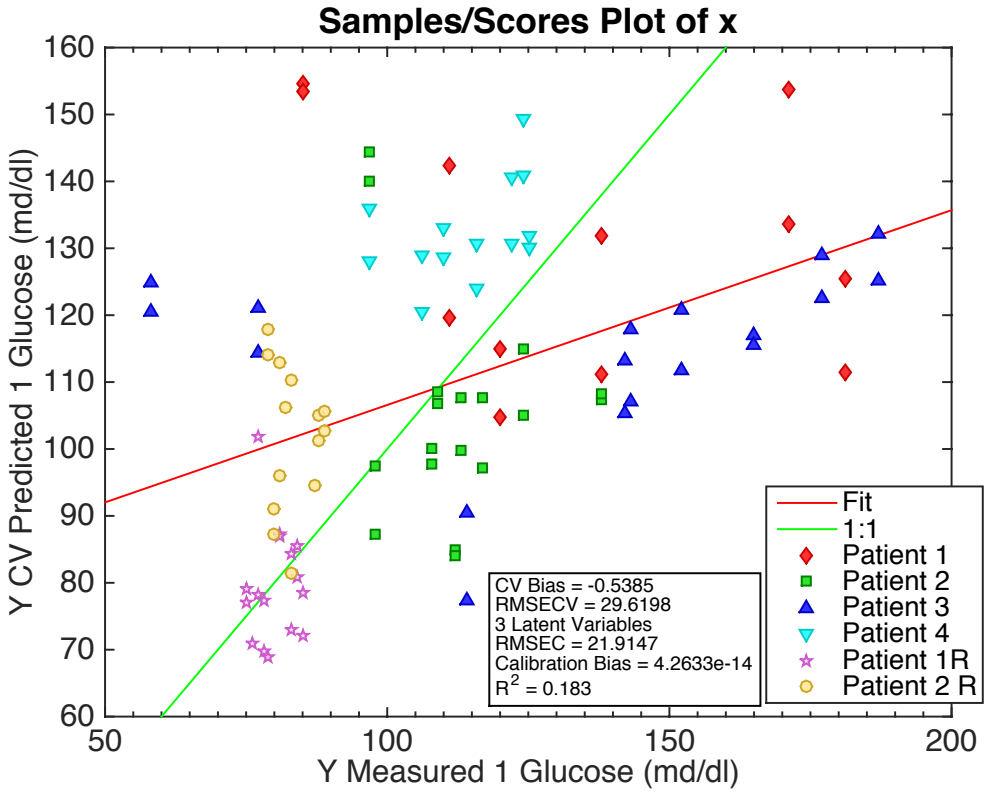
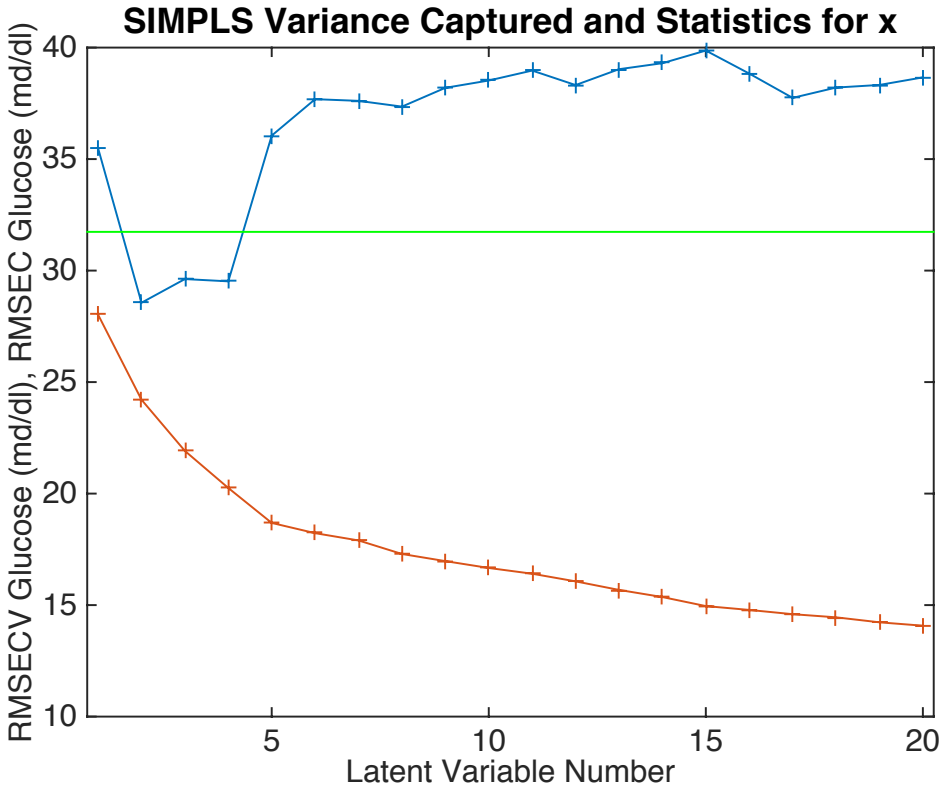
Best Model Patient CV





Cross-validation by patient (6 splits)

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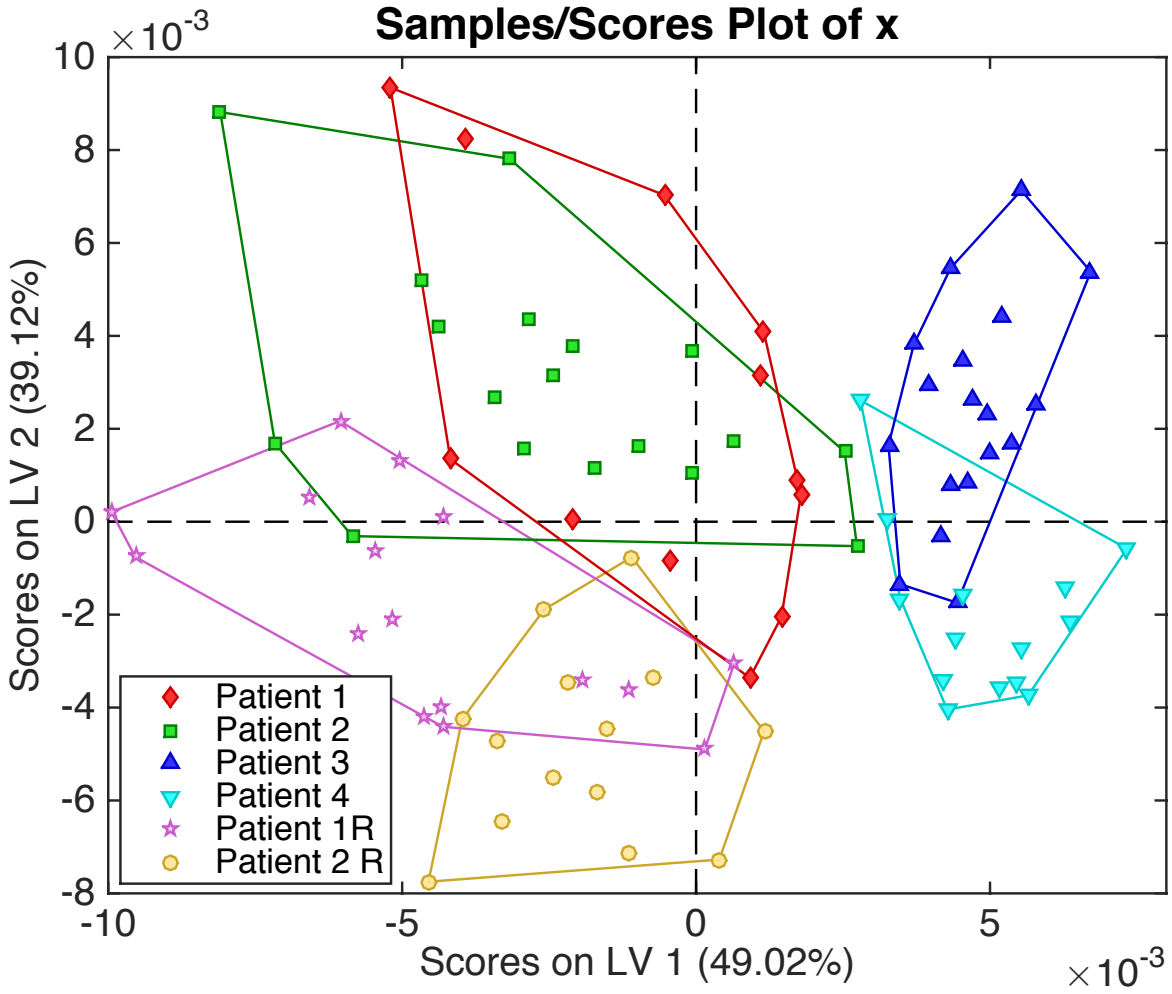
Scores in 1st Derivative Model



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Conclusions (IMHO)

- Preprocessing and variable selection
  - Can often make a good model better
  - Seldom make a bad model good
- Should be able to see signal in preprocessed data
  - At least in spectroscopy
  - Discrete variables maybe not
- Exhaustive search increases chance of false discovery – don't try too hard?
- Can be difficult to deal with clients
  - At what point do you tell them to give up?
- Still worry about missing something that works!