

Reimplementation of Lonnberg et al GPFates (from their example)

```
In [112]: import pandas as pd
import numpy as np
from GPfates import GPfates
import matplotlib.pyplot as plt
from scipy.linalg import svd
import GPy
```

Load in the expression data, filter and log normalize

```
In [35]: etpm = pd.read_table('tapio_tcell_tpm.txt', index_col=0)
etpm = etpm[(etpm > 2).sum(1) > 2]
logexp = np.log10(etpm + 1)
```

Load metadata

```
In [36]: tcells = pd.read_csv('tcells_rebuttal.csv', index_col=0)
```

Create a GPfates object

```
In [45]: mydata = GPfates.GPfates(sample_info=tcells, expression_matrix=logexp)
```

Use a GPLVM to infer a low-dimensional representation of the data

```
In [46]: mydata.dimensionality_reduction()

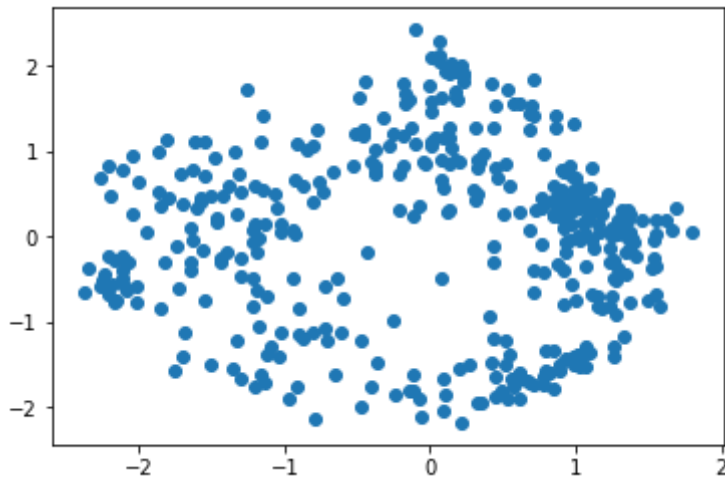
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:62: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

This is very cool. Their dimensionality reduction calls GPy.models.BayesianGPLVM - note to self, check that out. I am now going to store these results, overwriting the previous data they previously had stored in their metadata

```
In [47]: mydata.store_dr()
```

What does this dimensionality reduction look like?

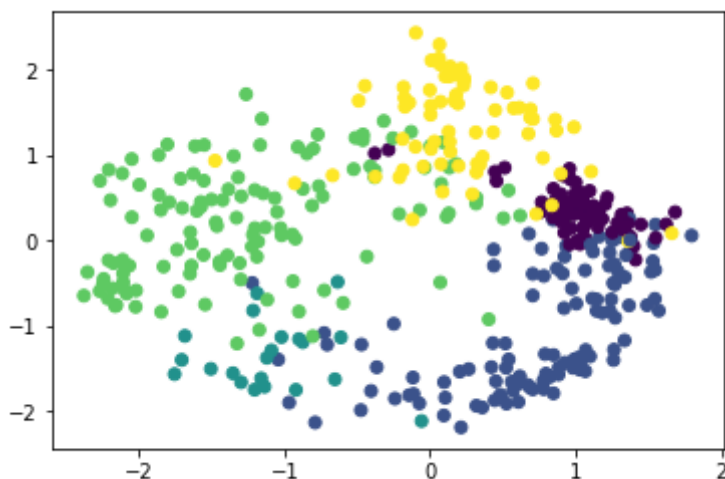
```
In [52]: dim1 = mydata.s['bgplvm_0']  
dim2 = mydata.s['bgplvm_1']  
plt.scatter(dim1, dim2)  
plt.show()
```



... neat? Try coloring by day

```
In [56]: fig, ax = plt.subplots()  
days = np.unique(mydata.s['day'])  
colors = np.linspace(0, 1, len(days))  
colordict = dict(zip(days, colors))  
  
day2col = mydata.s['day'].apply(lambda x: colordict[x])  
ax.scatter(dim1, dim2, c=day2col)  
fig.show()
```

/software/apps/anaconda/5.2/python/3.6/lib/python3.6/site-packages/matplotlib/figure.py:459: UserWarning:matplotlib is currently using a non-GUI backend, so cannot show the figure



Not going to worry about a legend here, but the color assignments are:

day 0: purple

day 2: dark blue

day 3: dark teal

day 4: green

day 7: yellow

So this is showing clear separation by day. How does this dimensionality reduction compare to what PCA would give us?

```
In [65]: mymat = mydata._gene_filter(None).as_matrix().T
u, s, vh = svd(mymat)
loadings = np.matmul(mymat, vh.T)

/software/apps/anaconda/5.2/python/3.6/lib/python3.6/site-packages/ipy
kernel/_main_.py:1: FutureWarning:Method .as_matrix will be removed i
n a future version. Use .values instead.
```

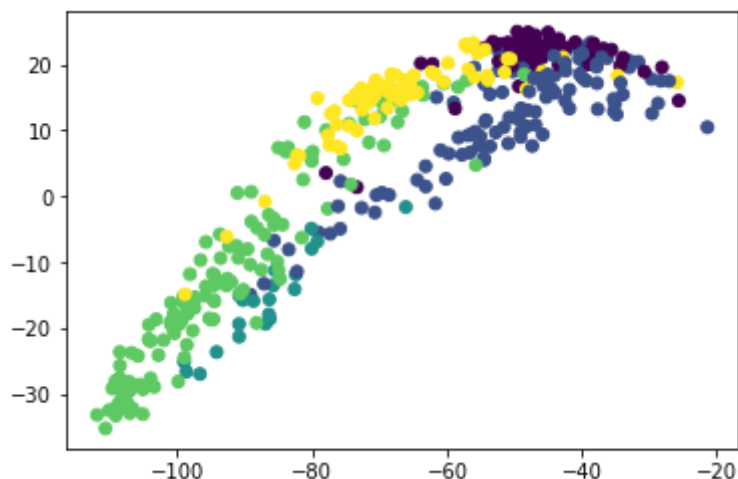
```
In [66]: loadings.shape
```

```
Out[66]: (408, 13931)
```

```
In [68]: fig, ax = plt.subplots()
days = np.unique(mydata.s['day'])
colors = np.linspace(0, 1, len(days))
colordict = dict(zip(days, colors))

day2col = mydata.s['day'].apply(lambda x: colordict[x])
ax.scatter(loadings[:,0], loadings[:,1], c=day2col)
fig.show()
```

```
/software/apps/anaconda/5.2/python/3.6/lib/python3.6/site-packages/mat
plotlib/figure.py:459: UserWarning:matplotlib is currently using a non-
GUI backend, so cannot show the figure
```



Interestingly enough it looks like PCA may capture the exact same trend as the GPLVM did, though maybe with slightly worse resolution. I don't have a great understanding of how the GPLVM works, but this is surprising to me. I'll read up about Gaussian processes and GPLVMs and think about whether this should be a surprising result, or if this is what we should expect. I'm going to store these results.

```
In [70]: mydata.s['pca_0'] = loadings[:,0]
         mydata.s['pca_1'] = loadings[:,1]
```

Infer pseudotime

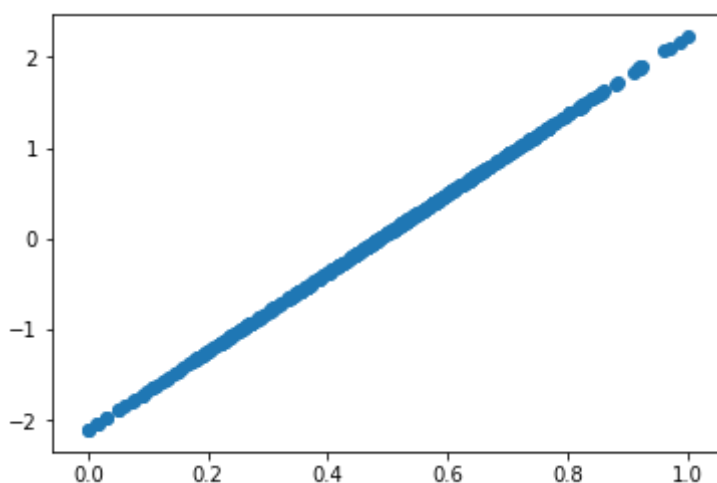
```
In [107]: mydata.infer_pseudotime(priors=mydata.s.day_int, s_columns=['bgplvm_0',
                           'bgplvm_1'])
```

```
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:36: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

This converged extremely quickly. At this point, they mention scaled_pseudotime, which I'm going to assume is just this inferred pseudotime scaled to be from zero to 1

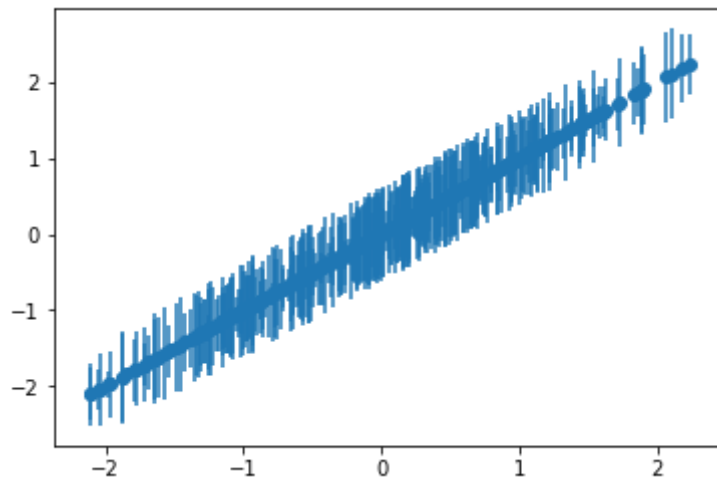
```
In [81]: mydata.s.scaled_pseudotime = mydata.s.pseudotime+abs(min(mydata.s.pseudotime))
         mydata.s.scaled_pseudotime = mydata.s.scaled_pseudotime/max(mydata.s.scaled_pseudotime)
```

```
In [83]: plt.scatter(mydata.s.scaled_pseudotime, mydata.s.pseudotime)
         plt.show()
```



I guess this is just meant to show what the scaling did? There's also a method to show uncertainty (psuedotime is their typo not mine)

```
In [91]: mydata.plot_pseudotime_uncertainty()
```



Now that we've inferred pseudotime, it's time to use the Overlapping Mixture of Gaussian Processes model to take a look at bifurcation - we assume that before bifurcation, the two processes are the same, and afterwards they are not

```
In [92]: mydata.model_fates(t='pseudotime', X=['bgplvm_0', 'bgplvm_1'], C=2, step  
_length=0.01)
```

```
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:79: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

```
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```



```
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```

```
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iteration 154 bound=-4950.517904382135 grad=3.8417725873228354e-05, bet
a=0.8061251962528427
iteration 155 bound=-4950.517901455748 grad=2.8955172934741732e-05, bet
a=0.7963187293387912
iteration 156 bound=-4950.517899282798 grad=2.198907038407713e-05, beta
=0.7911715867849152
iteration 157 bound=-4950.517897612343 grad=1.6882428798374607e-05, bet
a=0.7878687251706553
iteration 158 bound=-4950.517896289473 grad=1.3124839003332345e-05, bet
a=0.788095746172394
iteration 159 bound=-4950.517895249216 grad=1.032023715060535e-05, beta
=0.7896083646625445
iteration 160 bound=-4950.517894474029 grad=8.208187573759046e-06, beta
=0.785779654523825
vb converged (ftol)
```

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iteration 161 bound=-4827.990729709786 grad=240.48605306298174, beta=0.0
iteration 162 bound=-4825.809580774113 grad=152.87485321932056, beta=0.5653442766704981
iteration 163 bound=-4824.384181168376 grad=100.571260874551, beta=0.2949638308027061
iteration 164 bound=-4822.9234623825 grad=82.64412277025455, beta=0.5544385452625498
iteration 165 bound=-4821.542454818935 grad=69.62928389731593, beta=0.5504167753620569
iteration 166 bound=-4820.218653527341 grad=61.356522222225955, beta=0.5780469845479458
iteration 167 bound=-4818.900638099524 grad=55.51637774406234, beta=0.6321837344319674
iteration 168 bound=-4817.609251629951 grad=50.82626015494145, beta=0.6466897247378068
iteration 169 bound=-4816.3629185979735 grad=46.721744323700534, beta=0.6592248802736702
iteration 170 bound=-4815.178921440148 grad=42.6731591795307, beta=0.6738896646785315
iteration 171 bound=-4814.067552082694 grad=38.29253636211872, beta=0.699405156589156
iteration 172 bound=-4813.044564221097 grad=33.35446538045129, beta=0.7282762715728771
iteration 173 bound=-4812.14367714842 grad=27.916671245303064, beta=0.738119083998989
iteration 174 bound=-4811.3938237397815 grad=22.427464176156544, beta=0.7268330028556287
iteration 175 bound=-4810.797022036272 grad=17.52274308677719, beta=0.7055369770870251
iteration 176 bound=-4810.330548449431 grad=13.652279258893715, beta=0.6840796018456955
iteration 177 bound=-4809.963041856571 grad=10.914789087411938, beta=0.6643464654112204
iteration 178 bound=-4809.664959587181 grad=9.152521679155935, beta=0.648454475085925
iteration 179 bound=-4809.411364476437 grad=8.084351293640616, beta=0.6447875181032026
iteration 180 bound=-4809.181143860094 grad=7.417200652382047, beta=0.6672895991580826
iteration 181 bound=-4808.954729279635 grad=6.919227929377981, beta=0.7320675033632001
iteration 182 bound=-4808.71813434804 grad=6.433900730893402, beta=0.8171742370334266
iteration 183 bound=-4808.470458151924 grad=5.867980670742462, beta=0.8692476104904996
iteration 184 bound=-4808.223184225971 grad=5.186827377404751, beta=0.8765654643211305
iteration 185 bound=-4807.993279735632 grad=4.415489745341323, beta=0.8554832304524106
iteration 186 bound=-4807.794971091039 grad=3.6263312651942554, beta=0.88220873419382173
iteration 187 bound=-4807.634165370258 grad=2.9033301940492917, beta=0.7894741508122289
iteration 188 bound=-4807.508382441834 grad=2.3000679343009303, beta=0.7675793128155513
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```

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iteration 191 bound=-4807.274827408557 grad=1.1759150078742941, beta=0.
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iteration 192 bound=-4807.227116429017 grad=0.95947987255633, beta=0.75
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iteration 193 bound=-4807.188924409526 grad=0.7970166315876571, beta=0.
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iteration 194 bound=-4807.157920864102 grad=0.678721651592826, beta=0.7
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iteration 195 bound=-4807.13200141787 grad=0.5939321903930032, beta=0.7
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iteration 196 bound=-4807.10931699167 grad=0.531401476029423, beta=0.75
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iteration 197 bound=-4807.088430513435 grad=0.48136018975065764, beta=
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iteration 198 bound=-4807.068457286925 grad=0.4368940324984568, beta=0.
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iteration 199 bound=-4807.049079497718 grad=0.3940410762918706, beta=0.
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iteration 200 bound=-4807.030412947064 grad=0.3513511292746825, beta=0.
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iteration 201 bound=-4807.012789069326 grad=0.3092592790656896, beta=0.
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iteration 203 bound=-4806.98191908729 grad=0.23308319051761084, beta=0.
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iteration 204 bound=-4806.968925094605 grad=0.20187695550424695, beta=
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iteration 205 bound=-4806.9574481111 grad=0.17596252845853017, beta=0.8
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iteration 215 bound=-4806.882700970481 grad=0.08661286895881015, beta=
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```

```
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iteration 226 bound=-4806.842716025123 grad=0.09131080298080166, beta=
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iteration 231 bound=-4806.775060207621 grad=0.15168221030053783, beta=
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iteration 232 bound=-4806.745436288339 grad=0.1878114550891097, beta=1.
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iteration 233 bound=-4806.702906139551 grad=0.2438133345254053, beta=1.
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iteration 234 bound=-4806.6389667499325 grad=0.3329092790866728, beta=
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iteration 237 bound=-4806.121267797462 grad=1.0963549307924256, beta=1.
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iteration 238 bound=-4805.719082285511 grad=1.6658756094625016, beta=1.
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iteration 241 bound=-4804.9140310599705 grad=7.3207555721006905, beta=
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iteration 242 bound=-4804.59763101321 grad=7.3531861319561225, beta=3.3
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iteration 243 bound=-4803.591709306438 grad=8.064237268892045, beta=3.4
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iteration 247 bound=-4803.180997802874 grad=9.119712371485672, beta=0.2
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iteration 248 bound=-4803.051063802649 grad=8.429240351615661, beta=0.4
```



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iteration 249 bound=-4802.922243186947 grad=7.817020817592004, beta=0.4
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iteration 253 bound=-4802.314217108166 grad=5.1763539548190405, beta=0.
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iteration 260 bound=-4800.809990530191 grad=4.4764866704639505, beta=1.
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iteration 262 bound=-4797.197639306461 grad=11.677477789640148, beta=1.
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iteration 263 bound=-4791.9052291266835 grad=26.7384754962059, beta=3.6
7482766403953
iteration 265 bound=-4790.181611154506 grad=77.97421576325027, beta=1.0
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32964509642835
iteration 271 bound=-4787.327781134393 grad=22.179201637136465, beta=0.
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iteration 272 bound=-4786.979749520996 grad=18.031258482038535, beta=0.
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```

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iteration 280 bound=-4784.950701828616 grad=11.403295557900346, beta=1.
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iteration 303 bound=-4778.64581045277 grad=0.07826395494624755, beta=0.
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iteration 307 bound=-4778.631993987455 grad=0.031667916751039485, beta=
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iteration 308 bound=-4778.630002654368 grad=0.024224877062421137, beta=
```

```
0.8140315320807965
iteration 309 bound=-4778.628469991457 grad=0.0183979741796894, beta=0.7990092378897792
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iteration 311 bound=-4778.62640808246 grad=0.01070550819321191, beta=0.7868739519209315
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iteration 335 bound=-4778.6235042322305 grad=5.169296356144755e-05, beta=0.8030915820955111
iteration 336 bound=-4778.623501533303 grad=4.3405204408644716e-05, beta=0.8117662940298459
```

```
iteration 337 bound=-4778.623499234738 grad=3.6450707725820526e-05, bet
a=0.830377943226431
iteration 338 bound=-4778.623497204841 grad=3.0339597944318383e-05, bet
a=0.8401808675243814
iteration 339 bound=-4778.623495513604 grad=2.4931661796384467e-05, bet
a=0.838390934613671
iteration 340 bound=-4778.623494042315 grad=2.0273242743977314e-05, bet
a=0.8260357451927364
iteration 341 bound=-4778.623492864992 grad=1.647195406455814e-05, beta
=0.8075941448238982
iteration 342 bound=-4778.623491829306 grad=1.3500158084259006e-05, bet
a=0.8077832800867665
iteration 343 bound=-4778.623490994553 grad=1.1099952257090728e-05, bet
a=0.8292002180804428
vb converged (ftol)
```

```
/home-2/jpoppp4@jhu.edu/.local/lib/python3.6/site-packages/paramz/trans
formations.py:111: RuntimeWarning:overflow encountered in expm1
```

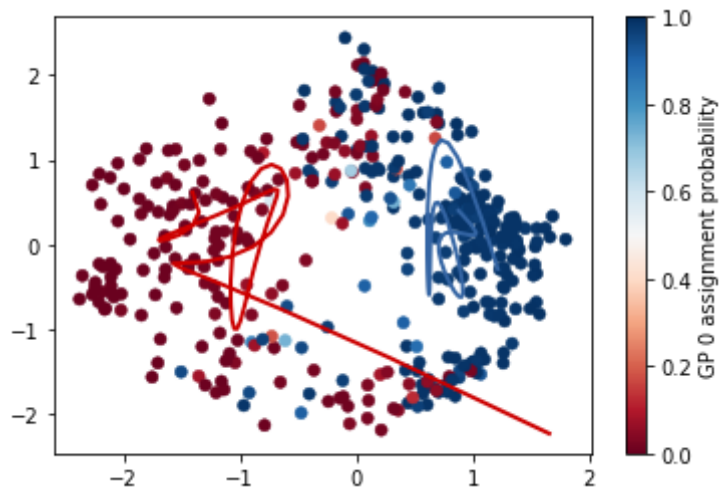
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iteration 347 bound=-4774.750341470815 grad=0.38261620377075317, beta=
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iteration 348 bound=-4774.745561991375 grad=0.26627814518087506, beta=
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iteration 352 bound=-4774.730774629364 grad=0.11175195013006728, beta=
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iteration 354 bound=-4774.725482117857 grad=0.07529850357073926, beta=
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iteration 355 bound=-4774.723257256915 grad=0.062229151549712376, beta=
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iteration 357 bound=-4774.719579443058 grad=0.04167046082689362, beta=
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iteration 358 bound=-4774.718088672674 grad=0.033991687911920636, beta=
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iteration 359 bound=-4774.716822419262 grad=0.02761615232002858, beta=
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iteration 360 bound=-4774.715760004935 grad=0.022506194651251223, beta=
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iteration 361 bound=-4774.714852928396 grad=0.018304558937577195, beta=
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iteration 362 bound=-4774.714088765348 grad=0.014662295563627132, beta=
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iteration 363 bound=-4774.713465586331 grad=0.011637691482283708, beta=
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iteration 364 bound=-4774.712958791198 grad=0.009273060080753777, beta=
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iteration 365 bound=-4774.712544715313 grad=0.007409676837738631, beta=
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iteration 366 bound=-4774.712210084837 grad=0.0059347235261063905, beta
=0.7785813843733345
iteration 367 bound=-4774.711940243178 grad=0.00479470251140386, beta=
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iteration 368 bound=-4774.711720665225 grad=0.003916676288477614, beta=
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iteration 370 bound=-4774.711387355482 grad=0.0026953425206595275, beta
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iteration 371 bound=-4774.711257443899 grad=0.002244466113511951, beta=
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iteration 372 bound=-4774.711147402533 grad=0.001859928818623581, beta=
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```

```
iteration 373 bound=-4774.711054475833 grad=0.0015343528932965187, beta=
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iteration 374 bound=-4774.710976299147 grad=0.001260284166964987, beta=
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iteration 375 bound=-4774.710910471455 grad=0.00103257272863652, beta=
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iteration 376 bound=-4774.710854739806 grad=0.0008424690210933713, beta=
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iteration 377 bound=-4774.7108078359515 grad=0.0006778098763413824, bet
a=0.8324861974025376
iteration 378 bound=-4774.710769815658 grad=0.0005358896728915324, beta
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iteration 379 bound=-4774.710739847629 grad=0.00042011784362788214, bet
a=0.8059057949105655
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=0.8079374944347433
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ta=0.7992670286691027
iteration 383 bound=-4774.710670705143 grad=0.00014838945521198358, bet
a=0.7968304721413009
iteration 384 bound=-4774.710661835397 grad=0.00011262454804210882, bet
a=0.7931243752163737
iteration 385 bound=-4774.710655251086 grad=8.521481085219604e-05, beta
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iteration 386 bound=-4774.710650371499 grad=6.449607030279103e-05, beta
=0.7836902306218767
iteration 387 bound=-4774.710646680567 grad=4.882451617776883e-05, beta
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iteration 388 bound=-4774.710643912396 grad=3.716118870904006e-05, beta
=0.7681192030830952
iteration 389 bound=-4774.710641735181 grad=2.871534693332499e-05, beta
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iteration 390 bound=-4774.710640144199 grad=2.2604973441038384e-05, bet
a=0.7635852900868292
iteration 391 bound=-4774.710638975299 grad=1.8088910691065264e-05, bet
a=0.7699350130740727
iteration 392 bound=-4774.710638146978 grad=1.4623116431127213e-05, bet
a=0.784076424109071
vb converged (ftol)
```

Visualize the results

```
In [94]: mydata.make_fates_viz(['bgplvm_0', 'bgplvm_1'])  
mydata.fates_viz.plot()  
plt.show()
```

/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:91: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.



This is not looking great. Running blindly through their example worked fine, so I'm going to do that to see where the discrepancy is.

```
In [102]: etpm = pd.read_table('tapio_tcell_tpm.txt', index_col=0)
etpm = etpm[(etpm > 2).sum(1) > 2]
logexp = np.log10(etpm + 1)
tcells = pd.read_csv('tcells_rebuttall.csv', index_col=0)
m = GPfates.GPfates(tcells, logexp)
m.model_fates(X=['bgplvm_2d_1'])
m.make_fates_viz(['bgplvm_2d_0', 'bgplvm_2d_1'])
m.fates_viz.plot()
GPfates.plt.show()
```



```
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:79: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

```
iteration 1 bound=622.9402548632543 grad=788.1552520657145, beta=0
iteration 2 bound=638.0418151074075 grad=719.9318102995865, beta=1.0074
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iteration 3 bound=659.1414905847172 grad=612.651839465461, beta=1.00623
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iteration 4 bound=684.1119154724732 grad=491.7901543669228, beta=0.9893
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iteration 5 bound=709.4269255704426 grad=371.42294155912793, beta=0.949
2073030422927
iteration 6 bound=730.9430728367795 grad=261.85483110202745, beta=0.886
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iteration 7 bound=746.2673669137845 grad=173.53227128904464, beta=0.815
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iteration 8 bound=755.7584035631436 grad=112.05397814005299, beta=0.755
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iteration 9 bound=761.191235817078 grad=74.57809230431087, beta=0.71215
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iteration 10 bound=764.2774793806259 grad=53.60389542717088, beta=0.685
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iteration 11 bound=766.159910016148 grad=42.09393669598432, beta=0.6790
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iteration 13 bound=768.5320257809867 grad=31.038577979684852, beta=0.73
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iteration 14 bound=769.4749760444419 grad=27.826844845865004, beta=0.77
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iteration 15 bound=770.3624727738481 grad=25.294151435323123, beta=0.79
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iteration 16 bound=771.2158147114421 grad=23.26481292182127, beta=0.797
0029517610858
iteration 17 bound=772.0364252698528 grad=21.682642623755385, beta=0.78
38782841814258
iteration 18 bound=772.8128785913362 grad=20.529296545357, beta=0.75241
34247111377
iteration 19 bound=773.5202372025643 grad=19.785712670670407, beta=0.69
3462761197384
iteration 20 bound=774.1040592199719 grad=19.412457784497434, beta=0.56
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iteration 21 bound=774.3200476068482 grad=19.339432585936756, beta=0.03
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iteration 22 bound=774.7598922307524 grad=19.444207638975804, beta=1.13
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iteration 23 bound=775.4951029891314 grad=19.700478397382838, beta=1.21
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iteration 24 bound=776.6452147162162 grad=20.208627953750845, beta=1.28
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iteration 25 bound=778.3891314655253 grad=21.121789503158247, beta=1.33
6107008128886
iteration 26 bound=780.9698902402233 grad=22.57523469972689, beta=1.390
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iteration 27 bound=784.6837903889977 grad=24.38722443849165, beta=1.506
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iteration 28 bound=789.7872809947667 grad=25.298562126559506, beta=2.39
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iteration 29 bound=790.0341013133102 grad=24.9280809532093, beta=0.0
iteration 30 bound=790.4977387028118 grad=24.00008074648933, beta=0.952
```

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iteration 32 bound=791.8123058360948 grad=20.210454536851252, beta=0.86
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iteration 33 bound=792.5241470944989 grad=17.97775364968896, beta=0.838
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iteration 34 bound=793.2104691573973 grad=15.832014243259497, beta=0.82
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iteration 36 bound=794.4444768297892 grad=12.039601140664749, beta=0.82
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```

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```

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```

```
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iteration 160 bound=798.4033606433181 grad=0.006724541918085546, beta=
0.895855320780493
iteration 161 bound=798.4049862786351 grad=0.005490027228005118, beta=
0.8904446999875444
iteration 162 bound=798.4063005028315 grad=0.004435210053039981, beta=
0.8851636522100707
iteration 163 bound=798.4073499539935 grad=0.0035469528556677362, beta=
0.8800191250021474
iteration 164 bound=798.4081779132403 grad=0.0028092220265038097, beta=
0.8750077424249584
iteration 165 bound=798.4088234355282 grad=0.0022044773691216367, beta=
0.8701180274466591
iteration 166 bound=798.4093208981049 grad=0.0017148466272140187, beta=
0.8653333287686606
iteration 167 bound=798.4096998947105 grad=0.0013230327273651091, beta=
0.86063486218093
iteration 168 bound=798.4099853920163 grad=0.0010129483680409264, beta=
0.8560042957237672
iteration 169 bound=798.4101980663349 grad=0.00077010474870248, beta=0.
8514255247707773
iteration 170 bound=798.4103547486941 grad=0.0005817981899377284, beta=
0.8468856605113776
iteration 171 bound=798.4104689202939 grad=0.0004371432511166222, beta=
0.8423756860172809
iteration 172 bound=798.4105512149085 grad=0.0003269980614518264, beta=
0.8378915584137971
```

```
iteration 173 bound=798.4106098981119 grad=0.00024382085769167894, beta=
=0.8334365933275104
iteration 174 bound=798.4106513043146 grad=0.0001814888416133511, beta=
0.8290256536010637
iteration 175 bound=798.4106802214427 grad=0.00013510285253801922, beta=
=0.8246909893810812
iteration 176 bound=798.4107002196923 grad=0.0001007945524701699, beta=
0.8204886823320451
iteration 177 bound=798.410713925529 grad=7.554700200162228e-05, beta=
0.8165037874957632
iteration 178 bound=798.4107232451286 grad=5.703472186416786e-05, beta=
0.8128517407059055
iteration 179 bound=798.4107295430733 grad=4.348564788205853e-05, beta=
0.8096736841982954
iteration 180 bound=798.4107337828202 grad=3.356482209788133e-05, beta=
0.8071242835706277
iteration 181 bound=798.4107366352605 grad=2.627814528803166e-05, beta=
0.8053524757257977
iteration 182 bound=798.410738561264 grad=2.0893846610055313e-05, beta=
0.8044782245781434
iteration 183 bound=798.4107398733605 grad=1.6879221991974003e-05, beta=
=0.8045709872747444
iteration 184 bound=798.4107407809807 grad=1.3850369687700668e-05, beta=
=0.805636689034423
vb converged (ftol)
```



```
iteration 185 bound=801.0907154156744 grad=0.3013936784696581, beta=0.0
iteration 186 bound=801.0960912504326 grad=0.2804749175401662, beta=0.9
488205791370193
iteration 187 bound=801.1028441307171 grad=0.24379041694413495, beta=0.
8993502050731204
iteration 188 bound=801.1098625328138 grad=0.20034014388393473, beta=0.
8536436582895548
iteration 189 bound=801.116327199823 grad=0.1588445155737386, beta=0.81
43702998686366
iteration 190 bound=801.1218549579237 grad=0.12454219552399909, beta=0.
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iteration 191 bound=801.1264200949432 grad=0.09859885407549857, beta=0.
7689202988685222
iteration 192 bound=801.1301801357488 grad=0.07958879158051674, beta=0.
7680850493372281
iteration 193 bound=801.1333258396753 grad=0.06536482418389261, beta=0.
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iteration 195 bound=801.138301777283 grad=0.04497714755682853, beta=0.8
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iteration 196 bound=801.1402688262167 grad=0.03725298151782141, beta=0.
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iteration 197 bound=801.141937806137 grad=0.03080881114145319, beta=0.8
052142948667572
iteration 198 bound=801.1433419587092 grad=0.025545907907852716, beta=
0.7990034722112488
iteration 199 bound=801.1445197593234 grad=0.02134677238427496, beta=0.
7935873615543196
iteration 200 bound=801.1455124015515 grad=0.01804500787138174, beta=0.
7915573933778927
iteration 201 bound=801.1463587213045 grad=0.015450455356328868, beta=
0.793682899961149
iteration 202 bound=801.147091259088 grad=0.013386965271331867, beta=0.
7988999835891787
iteration 203 bound=801.1477348834256 grad=0.011715590304691232, beta=
0.8051986410266683
iteration 204 bound=801.1483075986959 grad=0.01033812019036403, beta=0.
810926568012459
iteration 205 bound=801.1488223916035 grad=0.009188472067038638, beta=
0.8155731186585573
iteration 206 bound=801.1492890612018 grad=0.0082210184357806, beta=0.8
196257678023737
iteration 207 bound=801.149715461122 grad=0.007401487414548434, beta=0.
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iteration 208 bound=801.1501080732668 grad=0.0067021503537136005, beta=
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iteration 209 bound=801.1504721456897 grad=0.006100348027271752, beta=
0.8336113099956474
iteration 210 bound=801.1508117201716 grad=0.005578416824441662, beta=
0.8380643827523463
iteration 211 bound=801.1511297828332 grad=0.005123447858173792, beta=
0.8413806372726959
iteration 212 bound=801.151428594332 grad=0.004726266956579867, beta=0.
8435592278229016
iteration 213 bound=801.1517101053721 grad=0.004379862860416069, beta=
0.845292217078749
```

```
iteration 214 bound=801.1519763020028 grad=0.004077892908005157, beta=
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iteration 215 bound=801.1522293556011 grad=0.003813828717639308, beta=
0.8516123356932722
iteration 216 bound=801.152471542506 grad=0.0035809189536863033, beta=
0.8574379621677958
iteration 217 bound=801.1527050034751 grad=0.003372723564457041, beta=
0.8645875471822126
iteration 218 bound=801.1529314824985 grad=0.003183772748001071, beta=
0.8719426064876605
iteration 219 bound=801.1531521808463 grad=0.0030099785862031433, beta=
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iteration 220 bound=801.1533677906531 grad=0.0028486416373773226, beta=
0.8835977066143073
iteration 221 bound=801.1535786803531 grad=0.0026980987777454504, beta=
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iteration 222 bound=801.1537851384273 grad=0.002557190126031469, beta=
0.891715513002647
iteration 223 bound=801.1539875640063 grad=0.002424769218462312, beta=
0.8964259895125092
iteration 224 bound=801.1541865231611 grad=0.002299434816448954, beta=
0.9023555016662339
iteration 225 bound=801.1543826545338 grad=0.002179544824312853, beta=
0.9092758177058061
iteration 226 bound=801.1545764794068 grad=0.0020634458526994914, beta=
0.9163270221618073
iteration 227 bound=801.1547682126262 grad=0.0019497803906871661, beta=
0.9224260923626664
iteration 228 bound=801.1549576615829 grad=0.0018377336621021579, beta=
0.9267608684743158
iteration 229 bound=801.1551442515639 grad=0.0017271283088779212, beta=
0.9290907906335916
iteration 230 bound=801.1553271587549 grad=0.0016183392667310735, beta=
0.9297474186358035
iteration 231 bound=801.1555054920959 grad=0.0015120684156127925, beta=
0.9294121012281268
iteration 232 bound=801.1556784546772 grad=0.001409071231480182, beta=
0.9288124291479369
iteration 233 bound=801.1558454334204 grad=0.001309941223259615, beta=
0.9284574397861094
iteration 234 bound=801.1560060032144 grad=0.001215021226271555, beta=
0.9284952453742162
iteration 235 bound=801.1561598706479 grad=0.0011244432141368182, beta=
0.9287380896931089
iteration 236 bound=801.1563068044908 grad=0.0010382393287492395, beta=
0.9288383584686137
iteration 237 bound=801.1564465959455 grad=0.0009564461192906326, beta=
0.9285259301643162
iteration 238 bound=801.1565790661996 grad=0.0008791450541799813, beta=
0.9277834315109514
iteration 239 bound=801.1567041084363 grad=0.0008064276393099696, beta=
0.9268721939197223
iteration 240 bound=801.1568217318566 grad=0.0007383179670113517, beta=
0.9261999141780116
iteration 241 bound=801.1569320754447 grad=0.0006747075912770885, beta=
0.9260933413503598
iteration 242 bound=801.157035376903 grad=0.0006153475677242669, beta=
```

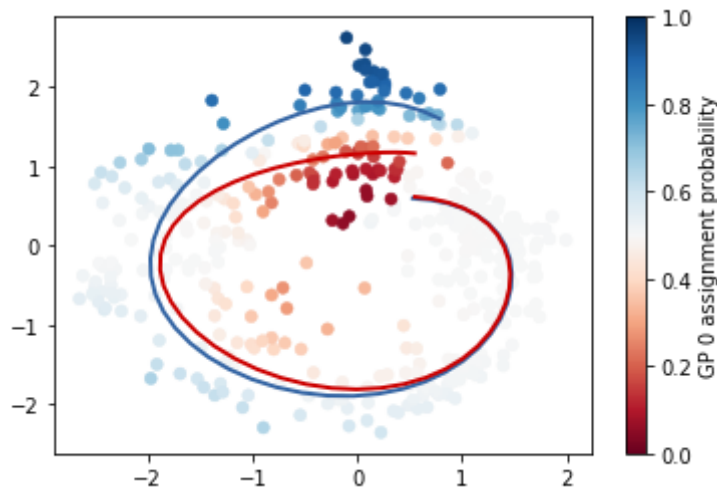
```
0.9265840106216235
iteration 243 bound=801.1571319076888 grad=0.0005599081947514425, beta=
0.927323398656673
iteration 244 bound=801.1572219043496 grad=0.0005080795184932012, beta=
0.927695294986885
iteration 245 bound=801.1573055288321 grad=0.00045966500075314196, beta
=0.9270872224572275
iteration 246 bound=801.1573828756573 grad=0.00041462435899744326, beta
=0.9251843694413958
iteration 247 bound=801.1574540208932 grad=0.0003730448442268074, beta=
0.922140525926178
iteration 248 bound=801.1575190890411 grad=0.00033505257171174556, beta
=0.9185582696966692
iteration 249 bound=801.1575783074371 grad=0.000300703534777786, beta=
0.9152961123982964
iteration 250 bound=801.1576320247099 grad=0.00026990367878504233, beta
=0.9131643707752172
iteration 251 bound=801.1576806861774 grad=0.00024239210108644688, beta
=0.9125970654807936
iteration 252 bound=801.1577247775726 grad=0.0002177892264724991, beta=
0.9134257647495662
iteration 253 bound=801.1577647611853 grad=0.0001956821425084797, beta=
0.9148971297591549
iteration 254 bound=801.1578010295732 grad=0.00017570801073478972, beta
=0.9159846919398916
iteration 255 bound=801.1578338915052 grad=0.00015760485021904148, beta
=0.9158564495266002
iteration 256 bound=801.1578635889168 grad=0.00014121739196741687, beta
=0.9142426411774586
iteration 257 bound=801.1578903313281 grad=0.00012646433035280573, beta
=0.9115282802186421
iteration 258 bound=801.1579143299883 grad=0.00011328664665525526, beta
=0.9085719574818488
iteration 259 bound=801.1579358180076 grad=0.00010160130844741852, beta
=0.9063595544353733
iteration 260 bound=801.1579550510228 grad=9.127869439041542e-05, beta=
0.9056181538958124
iteration 261 bound=801.1579722918768 grad=8.214837808887888e-05, beta=
0.9065180840305006
iteration 262 bound=801.157987788805 grad=7.402424421797182e-05, beta=
0.9085980910348963
iteration 263 bound=801.1580017573806 grad=6.6733679266191e-05, beta=0.
9109857061215708
iteration 264 bound=801.1580143727979 grad=6.013815202107178e-05, beta=
0.9128157111159804
iteration 265 bound=801.1580257730973 grad=5.413973613407299e-05, beta=
0.9136029992193286
iteration 266 bound=801.1580360691116 grad=4.867514096921901e-05, beta=
0.9133648089081934
iteration 267 bound=801.1580453554177 grad=4.3703060608490325e-05, beta
=0.9124720575694095
iteration 268 bound=801.1580537181003 grad=3.919156379569852e-05, beta=
0.9113624990955735
iteration 269 bound=801.158061237868 grad=3.511024492868897e-05, beta=
0.9102855870585537
iteration 270 bound=801.1580679898134 grad=3.142824286361589e-05, beta=
0.9092041799608196
```

```

iteration 271 bound=801.1580740422485 grad=2.8115992671508806e-05, beta=
=0.9078922558507376
iteration 272 bound=801.1580794566942 grad=2.5147293109987035e-05, beta=
=0.9061646825934879
iteration 273 bound=801.158084289666 grad=2.2499198192975316e-05, beta=
=0.9041012425965143
iteration 274 bound=801.1580885953997 grad=2.0149393787036934e-05, beta=
=0.9021298339542735
iteration 275 bound=801.1580924280307 grad=1.8072686419343334e-05, beta=
=0.9009053438419835
iteration 276 bound=801.1580958418717 grad=1.6238922819426454e-05, beta=
=0.9010144028569784
iteration 277 bound=801.1580988896069 grad=1.4613809505173855e-05, beta=
=0.9026267651784781
iteration 278 bound=801.1581016192335 grad=1.3162402236517862e-05, beta=
=0.9052861009701758
iteration 279 bound=801.1581040712516 grad=1.1853638566479064e-05, beta=
=0.9080165915195133
iteration 280 bound=801.1581062774967 grad=1.066393741160049e-05, beta=
=0.9097449026264491
iteration 281 bound=801.1581082620602 grad=9.578501447782435e-06, beta=
=0.9098021498826571
iteration 282 bound=801.1581100437412 grad=8.59000100348354e-06, beta=
=0.9082136676077254
iteration 283 bound=801.1581116389499 grad=7.695345803843171e-06, beta=
=0.9056527804306899
iteration 284 bound=801.1581130639222 grad=6.891962779561014e-06, beta=
=0.9031268614144754
iteration 285 bound=801.1581143356128 grad=6.17510582057254e-06, beta=
=0.9015391552598945
iteration 286 bound=801.1581154712719 grad=5.537108642321339e-06, beta=
=0.9012800357240888
iteration 287 bound=801.15811648721 grad=4.968468768864458e-06, beta=0.
9020184107364831
iteration 288 bound=801.1581173975476 grad=4.459830590338401e-06, beta=
=0.9028361841065322
vb converged (ftol)

```

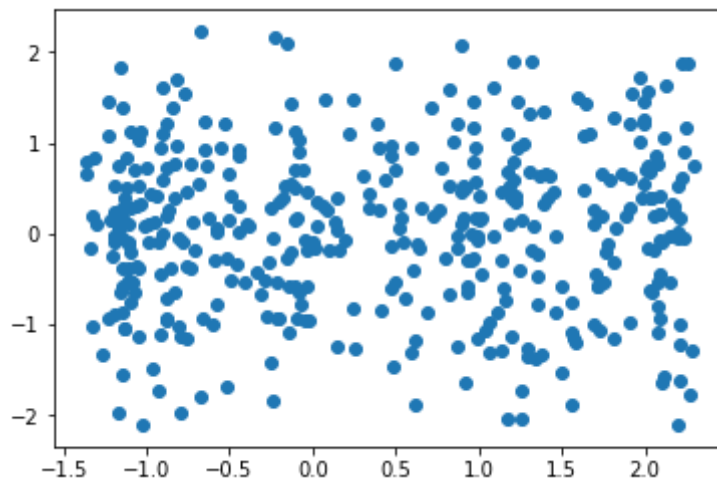
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:91: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.



```
In [104]: assert((m.s.day==mydata.s.day).all())
```

```
In [106]: plt.scatter(m.s.pseudotime, mydata.s.pseudotime)
```

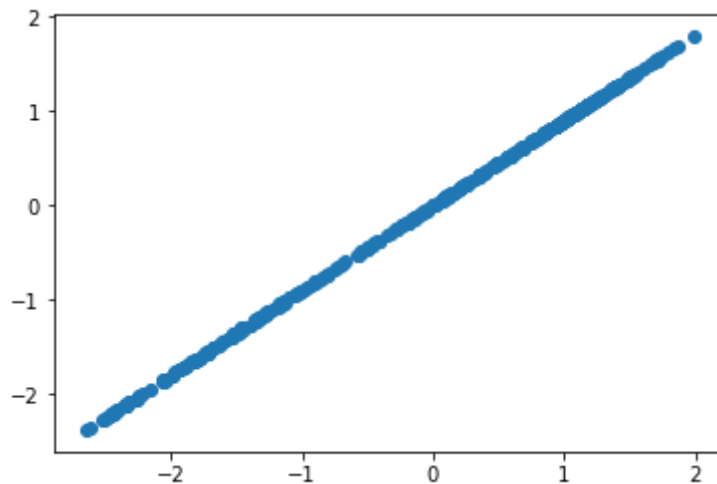
```
Out[106]: <matplotlib.collections.PathCollection at 0x2ae899bc9e80>
```



Well, that'll do it.

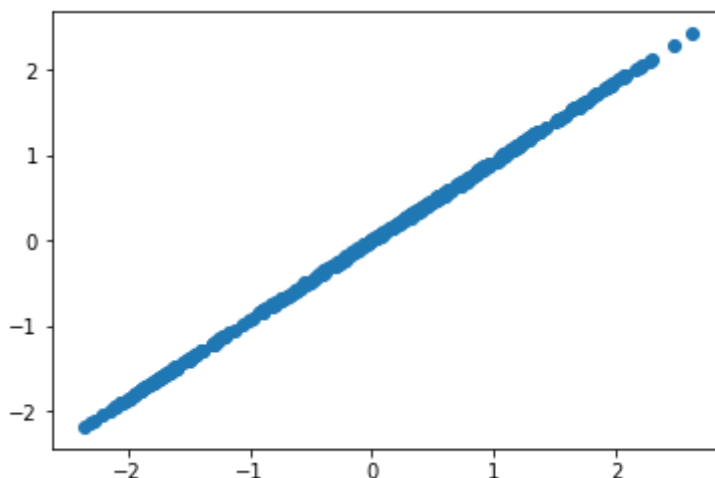
```
In [108]: plt.scatter(m.s.bgplvm_2d_0, mydata.s.bgplvm_0)
```

```
Out[108]: <matplotlib.collections.PathCollection at 0x2ae899c2ba58>
```



```
In [109]: plt.scatter(m.s.bgplvm_2d_1, mydata.s.bgplvm_1)
```

```
Out[109]: <matplotlib.collections.PathCollection at 0x2ae899c69cf8>
```



Considering how quickly pseudotime inference was converging, I think the error must be somewhere in pseudotime inference, because the dimensionality reduction being used is the same

```
In [119]: Y = mydata.s[['bgplvm_0', 'bgplvm_1']].as_matrix()

mydata.time_model = GPy.models.BayesianGPLVM(Y, 1, init='random')

mydata.time_model.rbf.lengthscale.constrain_fixed(2., warning=False)
mydata.time_model.rbf.variance.constrain_fixed(200., warning=False)

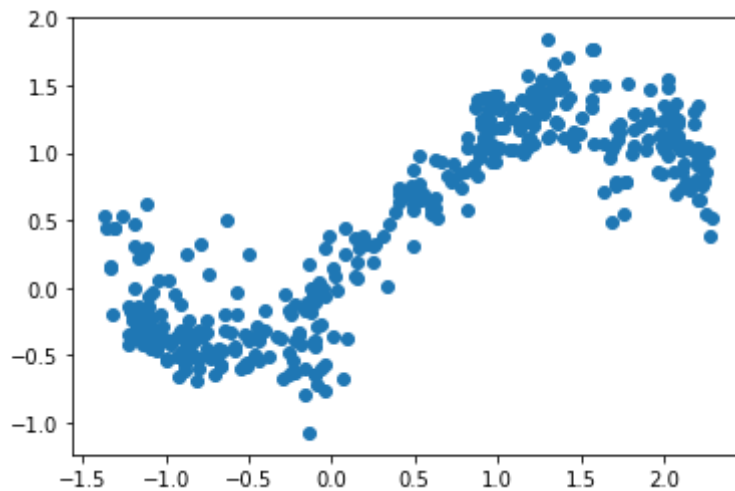
# priors = mydata.s.day_int+np.ones(len(mydata.s.day_int),dtype=int)
priors = mydata.s.day_int
if priors is not None:
    for i, p in enumerate(priors):
        prior = GPy.priors.Gaussian(p, 2.)
        mydata.time_model.X.mean[i, [0]].set_prior(prior, warning=False)

mydata.time_model.optimize(max_iters=2000, messages=True)
new_pseudotime = mydata.time_model.X.mean[:, [0]]

/software/apps/anaconda/5.2/python/3.6/lib/python3.6/site-packages/ipy
kernel/__main__.py:1: FutureWarning:Method .as_matrix will be removed i
n a future version. Use .values instead.
```

```
In [120]: plt.scatter(m.s.pseudotime, mydata.s.pseudotime)
```

```
Out[120]: <matplotlib.collections.PathCollection at 0x2ae899cbe2e8>
```



```
In [121]: Y = mydata.s[['bgplvm_0', 'bgplvm_1']].as_matrix()

mydata.time_model = GPy.models.BayesianGPLVM(Y, 1, init='random')

mydata.time_model.rbf.lengthscale.constrain_fixed(2., warning=False)
mydata.time_model.rbf.variance.constrain_fixed(200., warning=False)

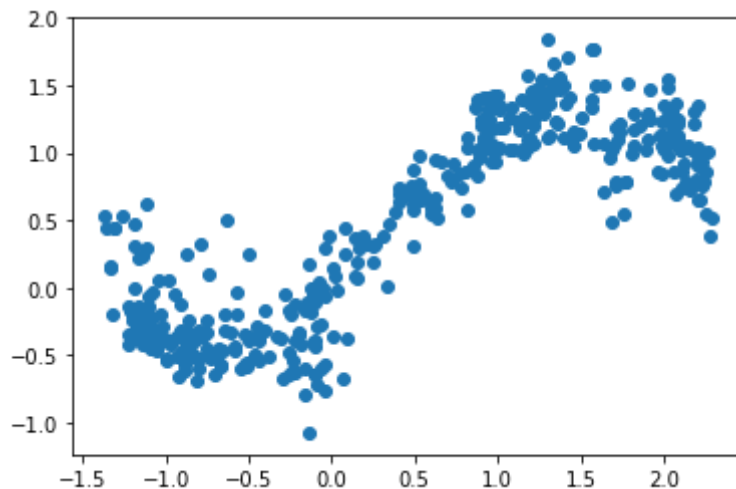
# priors = mydata.s.day_int+np.ones(len(mydata.s.day_int),dtype=int)
priors = mydata.s.day_int
if priors is not None:
    for i, p in enumerate(priors):
        prior = GPy.priors.Gaussian(p, 2.)
        mydata.time_model.X.mean[i, [0]].set_prior(prior, warning=False)

mydata.time_model.optimize(max_iters=2000, messages=True)
new_pseudotime2 = mydata.time_model.X.mean[:, [0]]

/software/apps/anaconda/5.2/python/3.6/lib/python3.6/site-packages/ipy
kernel/__main__.py:1: FutureWarning:Method .as_matrix will be removed i
n a future version. Use .values instead.
```

```
In [122]: plt.scatter(m.s.pseudotime, mydata.s.pseudotime)
```

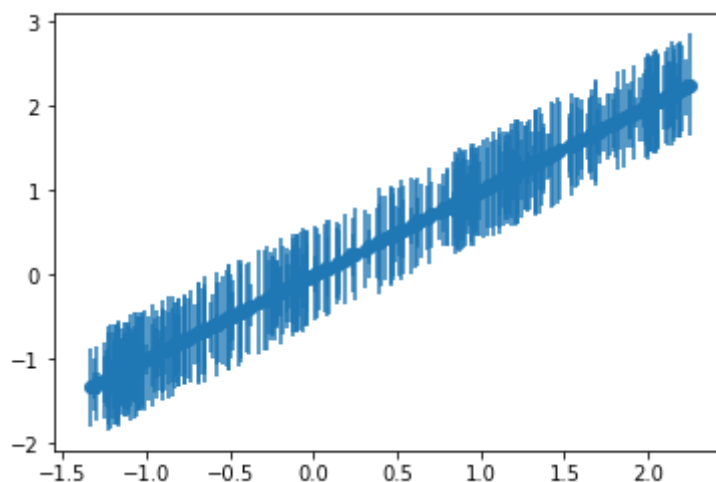
```
Out[122]: <matplotlib.collections.PathCollection at 0x2ae899dbfb38>
```



Now there's at least a relationship between the two pseudotime metrics, although I don't immediately know why the relationship would be sinusoidal. This seems like it'd have something to do with the fact that the pattern is circular. Traversing a unit circle, as x moves from 1 to 1 clockwise (like our data does with respect to latent component 1), y follows a sinusoidal pattern very much like this one. In their example where they don't actually do any learning, just using saved metadata, that metadata is labeled 'bgplvm_2d_0/1' rather than 'bgplvm_0/1' - I think there's some way to incorporate the two-dimensional nature of the data that I am not accounting for, but that'll have to wait until after my 4 hours. Either way, this should be better than the total randomness observed earlier. Does this improve results?

```
In [123]: mydata.s['pseudotime'] = new_pseudotime
mydata.s.scaled_pseudotime = mydata.s.pseudotime+abs(min(mydata.s.pseudotime))
mydata.s.scaled_pseudotime = mydata.s.scaled_pseudotime/max(mydata.s.scaled_pseudotime)
```

```
In [124]: mydata.plot_pseudotime_uncertainty()
```




```
In [125]: mydata.model_fates(t='pseudotime', X=['bgplvm_0', 'bgplvm_1'], C=2, step  
_length=0.01)
```

```
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:79: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

```
iteration 1 bound=612.7291215992004 grad=794.3169866361247, beta=0
iteration 2 bound=628.1808027447287 grad=686.5928435166828, beta=1.0675
921358749818
iteration 3 bound=649.0737952102413 grad=570.2033936100459, beta=1.0179
469399127892
iteration 4 bound=671.4131831046369 grad=454.1750731880182, beta=0.9583
798990687996
iteration 5 bound=693.0408779581926 grad=347.9366943163002, beta=0.9148
314568808406
iteration 6 bound=711.8006560655076 grad=258.7441969453073, beta=0.8817
15295660672
iteration 7 bound=725.0593097400468 grad=201.3643896105107, beta=0.7580
779323264336
iteration 8 bound=733.6506733549545 grad=159.5905612596406, beta=0.6805
075528209586
iteration 9 bound=740.7846405269111 grad=107.02603177556517, beta=0.922
4137559510245
iteration 10 bound=746.0906771501168 grad=64.93860342474652, beta=0.908
2348396866218
iteration 11 bound=749.2372886419614 grad=40.15191782795314, beta=0.794
0715801070295
iteration 12 bound=750.6444483707174 grad=27.361211397236602, beta=0.62
34812539987522
iteration 13 bound=751.2983360899151 grad=21.904219670073434, beta=0.54
68911406476158
iteration 14 bound=751.765425403032 grad=19.383397460220742, beta=0.647
1137868683734
iteration 15 bound=752.2063146326759 grad=17.56799532114322, beta=0.769
5252162168759
iteration 16 bound=752.6575447439293 grad=15.850191673464519, beta=0.83
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iteration 17 bound=753.1202164152105 grad=14.106418719618663, beta=0.86
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vb converged (ftol)
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iteration 221 bound=800.8067892150387 grad=36.2060002305812, beta=0.826
6416391055578
iteration 222 bound=801.6078362345235 grad=24.26132019698599, beta=0.68
7138587191103
iteration 223 bound=802.1501248034508 grad=18.69464894789553, beta=0.59
69981147991847
iteration 224 bound=802.5903778410791 grad=16.293734310570443, beta=0.6
349714273606047
iteration 225 bound=803.0192200918266 grad=14.832797932547583, beta=0.7
367327694763639
iteration 226 bound=803.4655306640009 grad=13.553591920145855, beta=0.8
091330713605617
iteration 227 bound=803.9294167249255 grad=12.267901428794634, beta=0.8
420081100075861
iteration 228 bound=804.398606810637 grad=10.968486692933416, beta=0.85
01113967732993
iteration 229 bound=804.8574248719506 grad=9.71136630991867, beta=0.845
0320240716431
iteration 230 bound=805.2924919449971 grad=8.563571875003358, beta=0.83
40646363337153
iteration 231 bound=805.6957124415962 grad=7.573329333653259, beta=0.82
20446724663192
iteration 232 bound=806.0647717652528 grad=6.757649988995885, beta=0.81
23656320115789
iteration 233 bound=806.4019157083945 grad=6.1050182610052115, beta=0.8
072615644426728
iteration 234 bound=806.712031999465 grad=5.586838493266374, beta=0.807
6687892419536
iteration 235 bound=807.0008412783432 grad=5.1698575228327694, beta=0.8
130721432967749
iteration 236 bound=807.2736294550814 grad=4.824484296838272, beta=0.82
1829019386003
iteration 237 bound=807.5346335358552 grad=4.528032018823344, beta=0.83
20638932224591
iteration 238 bound=807.7869574005149 grad=4.2644918570522945, beta=0.8
425214186556366
iteration 239 bound=808.0327602970121 grad=4.022886004884971, beta=0.85
27276141115864
iteration 240 bound=808.2734669345356 grad=3.795566473439528, beta=0.86
25330271690638
iteration 241 bound=808.509866796432 grad=3.5770372264163495, beta=0.87
16172431308393
iteration 242 bound=808.7421095330789 grad=3.3633615816511417, beta=0.8
793637518629913
iteration 243 bound=808.9696826215193 grad=3.151977469344143, beta=0.88
50807562905911
iteration 244 bound=809.1914600803736 grad=2.9416858697810433, beta=0.8
883142633370855
iteration 245 bound=809.4058661714878 grad=2.732610984690553, beta=0.88
9046269351797
```

```
iteration 246 bound=809.6111394380841 grad=2.5260019145563404, beta=0.8
877135424198526
iteration 247 bound=809.8056339479123 grad=2.323840293700108, beta=0.88
50794307068383
iteration 248 bound=809.9880740495046 grad=2.1283233683458445, beta=0.8
820233904345512
iteration 249 bound=810.1576952559695 grad=1.9413694058800488, beta=0.8
793137857632316
iteration 250 bound=810.3142491305937 grad=1.764297403010749, beta=0.87
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iteration 251 bound=810.4579010506947 grad=1.597757372076187, beta=0.87
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iteration 252 bound=810.589081559003 grad=1.4418758051323461, beta=0.87
61537383241159
iteration 253 bound=810.7083525883236 grad=1.2964993372680775, beta=0.8
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iteration 254 bound=810.8163248804117 grad=1.1614070868290902, beta=0.8
760195077917144
iteration 255 bound=810.9136297490957 grad=1.0364111484263132, beta=0.8
75664813399731
iteration 256 bound=811.0009241886168 grad=0.9213383784902187, beta=0.8
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iteration 257 bound=811.0789013806216 grad=0.8159458289994322, beta=0.8
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iteration 258 bound=811.1482867338732 grad=0.7198430590732474, beta=0.8
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iteration 259 bound=811.2098145852681 grad=0.6324750500458725, beta=0.8
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iteration 260 bound=811.2641939310485 grad=0.5531772611888177, beta=0.8
75786444978899
iteration 261 bound=811.3120774724222 grad=0.48127529372614647, beta=0.
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iteration 262 bound=811.3540458552486 grad=0.416183940572454, beta=0.87
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iteration 263 bound=811.390611257066 grad=0.3574665545155205, beta=0.87
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iteration 264 bound=811.4222361613805 grad=0.3048363775649017, beta=0.8
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iteration 265 bound=811.4493580500869 grad=0.2581050690761256, beta=0.8
71587908410265
iteration 266 bound=811.4724102104312 grad=0.21710174645887118, beta=0.
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iteration 267 bound=811.4918320319196 grad=0.1815937154318488, beta=0.8
640842711298128
iteration 268 bound=811.5080670429362 grad=0.15123612483516638, beta=0.
8603383767024506
iteration 269 bound=811.5215513883577 grad=0.1255642060432546, beta=0.8
572230760967305
iteration 270 bound=811.5326980104029 grad=0.10402464710785156, beta=0.
8550242813920834
iteration 271 bound=811.541882032433 grad=0.08602956841842829, beta=0.8
53775704757663
iteration 272 bound=811.5494312506751 grad=0.0710124285284519, beta=0.8
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iteration 273 bound=811.5556232253463 grad=0.05846976356680731, beta=0.
8529830513254103
iteration 274 bound=811.5606882319419 grad=0.047981657055374674, beta=
```

```
0.85250099181579
iteration 275 bound=811.5648159520599 grad=0.03921229876112779, beta=0.
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iteration 276 bound=811.5681634488809 grad=0.031897069952180196, beta=
0.8494509896779823
iteration 277 bound=811.5708624681229 grad=0.025823972498255354, beta=
0.846719553195901
iteration 278 bound=811.5730250084584 grad=0.02081596221147738, beta=0.
8434151358421582
iteration 279 bound=811.5747469895327 grad=0.016718144229606678, beta=
0.8398437115428103
iteration 280 bound=811.5761104412319 grad=0.013390935160038043, beta=
0.8362911041637962
iteration 281 bound=811.5771848634733 grad=0.010708055463905028, beta=
0.8329408229500035
iteration 282 bound=811.5780283248255 grad=0.008557114914949523, beta=
0.8298412972837446
iteration 283 bound=811.578688628437 grad=0.006840632022612725, beta=0.
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iteration 284 bound=811.579204624787 grad=0.005476165456641041, beta=0.
8241323433618225
iteration 285 bound=811.5796075880722 grad=0.00439523425735164, beta=0.
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iteration 286 bound=811.5799225234763 grad=0.003541408928073211, beta=
0.8189357137945403
iteration 287 bound=811.5801693048667 grad=0.002868204397697944, beta=
0.816964449417328
iteration 288 bound=811.5803636104599 grad=0.0023372806919287345, beta=
0.8158902401633582
iteration 289 bound=811.5805176773329 grad=0.0019171553754586616, beta=
0.8160461918406815
iteration 290 bound=811.5806409225092 grad=0.0015823499095270884, beta=
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iteration 291 bound=811.5807404755827 grad=0.0013127504401646945, beta=
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iteration 292 bound=811.5808216504921 grad=0.00109297775841595, beta=0.
8234517793086449
iteration 293 bound=811.5808883654181 grad=0.0009116654357686424, beta=
0.8266165430697184
iteration 294 bound=811.5809435060269 grad=0.0007606538696165046, beta=
0.8290556155705047
iteration 295 bound=811.5809892258162 grad=0.000634171053187645, beta=
0.8303903488119008
iteration 296 bound=811.5810271761844 grad=0.0005280847343555797, beta=
0.8305761833838992
iteration 297 bound=811.5810586703785 grad=0.00043929380406622067, beta
=0.8298543678291238
iteration 298 bound=811.5810847889672 grad=0.0003652954671111557, beta=
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iteration 299 bound=811.5811064412378 grad=0.0003039283305761058, beta=
0.8272863583990597
iteration 300 bound=811.5811243983101 grad=0.00025325843373853296, beta
=0.8261245195017183
iteration 301 bound=811.5811393112117 grad=0.0002115552423606542, beta=
0.8252315610076221
iteration 302 bound=811.5811517243881 grad=0.0001773034937943117, beta=
0.8245336800411456
```

```
iteration 303 bound=811.5811620887403 grad=0.00014921184459907967, beta=
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iteration 304 bound=811.5811707760287 grad=0.00012620107981158325, beta=
=0.8232275168850666
iteration 305 bound=811.5811780929969 grad=0.00010737331913652098, beta=
=0.8226717732371993
iteration 306 bound=811.5811842938633 grad=9.197367917544098e-05, beta=
0.8225783622718206
iteration 307 bound=811.5811895899155 grad=7.935687203117117e-05, beta=
0.82347029949526
iteration 308 bound=811.5811941560753 grad=6.896612426137395e-05, beta=
0.8258618026512918
iteration 309 bound=811.5811981352102 grad=6.032477183250275e-05, beta=
0.830022605416384
iteration 310 bound=811.5812016412533 grad=5.303565218507575e-05, beta=
0.8357783684287499
iteration 311 bound=811.5812047617442 grad=4.678191196390206e-05, beta=
0.8424666108562872
iteration 312 bound=811.5812075610526 grad=4.132456574345684e-05, beta=
0.8491093277199604
iteration 313 bound=811.581210084511 grad=3.649504705216514e-05, beta=
0.8547321057921023
iteration 314 bound=811.5812123631073 grad=3.218325712327853e-05, beta=
0.8586662055280241
iteration 315 bound=811.5812144183391 grad=2.8322730404260143e-05, beta=
=0.8607032955113297
iteration 316 bound=811.5812162663786 grad=2.487493008440943e-05, beta=
0.8610826856647437
iteration 317 bound=811.5812179218115 grad=2.1814809415748878e-05, beta=
=0.8603689654626577
iteration 318 bound=811.5812193993972 grad=1.9119602966305308e-05, beta=
=0.8592863206707952
iteration 319 bound=811.5812207151516 grad=1.676213678079537e-05, beta=
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iteration 320 bound=811.5812218857567 grad=1.4708805583645942e-05, beta=
=0.8587127166525294
iteration 321 bound=811.5812229281285 grad=1.2921183905644479e-05, beta=
=0.8600525237318806
iteration 322 bound=811.5812238580537 grad=1.1359533589438917e-05, beta=
=0.8625183455534824
vb converged (ftol)
```

```
iteration 323 bound=811.760187508413 grad=0.13371537628914235, beta=81
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iteration 324 bound=811.7617503482641 grad=0.15865952213362033, beta=0.
0
iteration 325 bound=811.7645993233812 grad=0.14847277855376304, beta=0.
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iteration 326 bound=811.7682094792852 grad=0.13059538949716093, beta=0.
8984056971322687
iteration 327 bound=811.7720162937204 grad=0.1093556554917627, beta=0.8
539270372382607
iteration 328 bound=811.7756000117745 grad=0.08888222907670296, beta=0.
8177040095720087
iteration 329 bound=811.7787549662444 grad=0.0716050366111002, beta=0.7
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iteration 330 bound=811.7814491211577 grad=0.058064290691376357, beta=
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iteration 331 bound=811.783738883558 grad=0.047661269478814286, beta=0.
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iteration 332 bound=811.7856980827734 grad=0.03951319236037044, beta=0.
7934846340980001
iteration 333 bound=811.7873840193695 grad=0.03292722619422681, beta=0.
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iteration 334 bound=811.7888340148443 grad=0.027499990559149735, beta=
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iteration 335 bound=811.7900751500761 grad=0.023031759003209973, beta=
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iteration 336 bound=811.7911336629905 grad=0.01940475076815048, beta=0.
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iteration 337 bound=811.7920384901639 grad=0.01650076068060826, beta=0.
7976575140094293
iteration 338 bound=811.7928194518964 grad=0.014178486595646921, beta=
0.8008425614368212
iteration 339 bound=811.793503221872 grad=0.012292275110360651, beta=0.
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iteration 340 bound=811.7941101788279 grad=0.01071975653770516, beta=0.
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iteration 345 bound=811.7963230814776 grad=0.005631106972961217, beta=
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iteration 346 bound=811.7966399763498 grad=0.005018018188406742, beta=
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iteration 347 bound=811.7969282947918 grad=0.004494133721328172, beta=
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iteration 348 bound=811.7971931772745 grad=0.004037373513998637, beta=
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iteration 349 bound=811.797438338489 grad=0.003630153213180958, beta=0.
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iteration 350 bound=811.7976660411275 grad=0.00326076157915276, beta=0.
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iteration 351 bound=811.797877491601 grad=0.0029226316882599883, beta=
```

```
0.8680416747907145
iteration 352 bound=811.7980733744391 grad=0.002612460628927219, beta=
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iteration 353 bound=811.7982542666787 grad=0.0023282458725740066, beta=
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iteration 354 bound=811.7984208048404 grad=0.0020680301893749482, beta=
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iteration 355 bound=811.7985736353476 grad=0.0018296211794640504, beta=
0.8785718083440871
iteration 356 bound=811.7987132847006 grad=0.0016110099301964915, beta=
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iteration 358 bound=811.7989542916779 grad=0.0012290871613482187, beta=
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iteration 360 bound=811.7991462257859 grad=0.0009213558520147993, beta=
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iteration 363 bound=811.7993552740895 grad=0.0005903942854596233, beta=
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iteration 365 bound=811.7994550402514 grad=0.000431465778853707, beta=
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iteration 366 bound=811.799495619401 grad=0.00036392992763601366, beta=
0.8825437283173393
iteration 367 bound=811.7995305894584 grad=0.0003032281127942618, beta=
0.8800077121781876
iteration 368 bound=811.7995602700987 grad=0.000249468672928979, beta=
0.8734569691057699
iteration 369 bound=811.7995850282603 grad=0.00020302824858674595, beta=
0.8641852024752913
iteration 370 bound=811.7996053429611 grad=0.00016409010810976795, beta=
0.8541519300407642
iteration 371 bound=811.7996217995097 grad=0.00013235727374050595, beta=
0.8454027308897095
iteration 372 bound=811.7996350335263 grad=0.00010703468969169578, beta=
0.8394842900613283
iteration 373 bound=811.7996456582546 grad=8.702636188346303e-05, beta=
0.8369120377696675
iteration 374 bound=811.7996542087125 grad=7.119914802048409e-05, beta=
0.8369411873067992
iteration 375 bound=811.7996611174981 grad=5.8578607519148764e-05, beta=
0.8379647995721419
iteration 376 bound=811.7996667197772 grad=4.8424180534337557e-05, beta=
0.8384769278029982
iteration 377 bound=811.7996712744864 grad=4.0206149929864e-05, beta=0.
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iteration 378 bound=811.7996749869694 grad=3.353814478975785e-05, beta=
0.8371702937760422
iteration 379 bound=811.7996780249384 grad=2.8113361486274907e-05, beta=
0.8373994641136685
```



```

iteration 380 bound=811.799680525923 grad=2.3669643316142378e-05, beta=
0.839629293695068
iteration 381 bound=811.7996825995381 grad=1.9983629385461894e-05, beta
=0.8436080786429118
iteration 382 bound=811.799684329364 grad=1.687889816244994e-05, beta=
0.8477773579394488
iteration 383 bound=811.7996857766884 grad=1.4231861371508297e-05, beta
=0.8501248430130088
iteration 384 bound=811.7996869864276 grad=1.1967007147124746e-05, beta
=0.849390849231977
iteration 385 bound=811.7996879938785 grad=1.0041823582431597e-05, beta
=0.8457835377864468
iteration 386 bound=811.7996888298226 grad=8.427347070984388e-06, beta=
0.8409028514562867
vb converged (ftol)

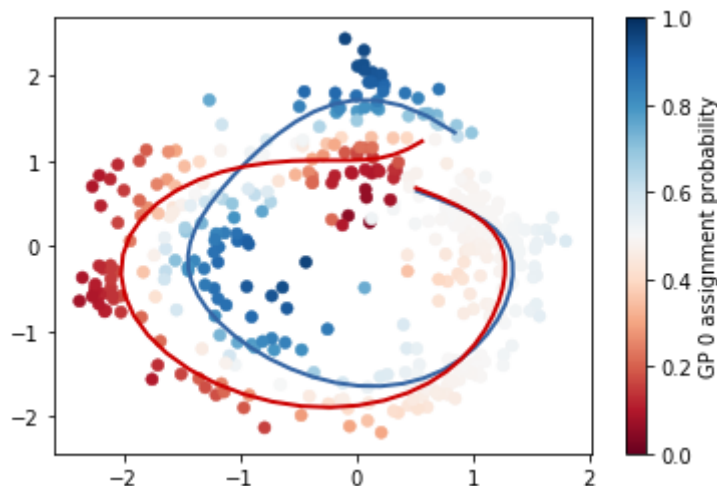
```

```

In [126]: mydata.make_fates_viz(['bgplvm_0', 'bgplvm_1'])
mydata.fates_viz.plot()
plt.show()

```

/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:91: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.



WOOHOO!! We have trajectories. They seem to bifurcate somewhat prematurely, but this looks pretty good overall. Many questions to dig into, but I believe my big problems came from the `infer_pseudotime` method being far from robust. Running it several times, I sometimes ran into errors, sometimes saw it converge immediately, etc. I think that is the reason the first results were essentially garbage. Why my inferred pseudotime is a sinusoidal transformation of theirs, and where they got their `bgplvm_2d` latent variables, I will need to think about to figure out. One last question - does PCA work for trajectory inference?

```
In [129]: Y = mydata.s[['pca_0', 'pca_1']].as_matrix()

mydata.time_model = GPy.models.BayesianGPLVM(Y, 1, init='random')

mydata.time_model.rbf.lengthscale.constrain_fixed(2., warning=False)
mydata.time_model.rbf.variance.constrain_fixed(200., warning=False)

# priors = mydata.s.day_int*np.ones(len(mydata.s.day_int),dtype=int)
priors = mydata.s.day_int
if priors is not None:
    for i, p in enumerate(priors):
        prior = GPy.priors.Gaussian(p, 2.)
        mydata.time_model.X.mean[i, [0]].set_prior(prior, warning=False)

mydata.time_model.optimize(max_iters=2000, messages=True)
mydata.s['pca_pseudotime'] = mydata.time_model.X.mean[:, [0]]
mydata.s['scaled_pca_pseudotime'] = mydata.s.pca_pseudotime+abs(min(mydata.s.pca_pseudotime))
mydata.s.scaled_pca_pseudotime = mydata.s.scaled_pca_pseudotime/max(mydata.s.scaled_pca_pseudotime)
mydata.model_fates(t='pca_pseudotime', X=['pca_0', 'pca_1'], C=2, step_length=0.01)
mydata.make_fates_viz(['pca_0', 'pca_1'])
mydata.fates_viz.plot()
plt.show()
```

```
/software/apps/anaconda/5.2/python/3.6/lib/python3.6/site-packages/ipykernel/__main__.py:1: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

```
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:79: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```

```
iteration 1 bound=-259948.12693189978 grad=429543.8626277946, beta=0
iteration 2 bound=-134714.57391608864 grad=25651835.295126826, beta=11.
050191627254565
iteration 3 bound=-122974.948897559 grad=4192037.882654677, beta=0.0
iteration 4 bound=-119262.41276722432 grad=23706740.787014797, beta=0.0
iteration 6 bound=-122962.76769021216 grad=10297425.926616227, beta=0.0
iteration 7 bound=-121402.90400990288 grad=33993761.67698123, beta=0.0
iteration 8 bound=-109888.17665712361 grad=15287752.625584178, beta=0.0
iteration 10 bound=-110547.3222258641 grad=2305852.6839771215, beta=0.0
iteration 11 bound=-105923.2618571575 grad=8366787.760247212, beta=0.0
iteration 13 bound=-106834.04289939435 grad=298936.2862746454, beta=0.0
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iteration 764 bound=-111742.37480075506 grad=2265494.725236354, beta=0.
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iteration 765 bound=-105238.38016690365 grad=15497816.573340494, beta=
0.0
iteration 767 bound=-105301.7174521167 grad=286766.19405153295, beta=0.
0
iteration 769 bound=-111893.98186156189 grad=1647805.7887281582, beta=
0.0
iteration 770 bound=-107233.85351594565 grad=10091827.718501236, beta=
```

```
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iteration 771 bound=-106651.39905746638 grad=10672300.343556501, beta=
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iteration 773 bound=-107220.49290991887 grad=7995460.2566401055, beta=
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iteration 775 bound=-107826.68070541607 grad=10384209.147682007, beta=
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iteration 777 bound=-108229.391487227 grad=10532136.725394627, beta=0.0
iteration 778 bound=-107846.46301643859 grad=13474203.902756386, beta=
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iteration 780 bound=-109924.50314598194 grad=10773922.88526636, beta=0.
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iteration 781 bound=-106455.31450972604 grad=12952294.63130237, beta=0.
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iteration 783 bound=-108251.11086313978 grad=7676616.452722522, beta=0.
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iteration 785 bound=-108668.40666905775 grad=11641534.140926208, beta=
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iteration 787 bound=-109886.96323555149 grad=13241378.308990184, beta=
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iteration 788 bound=-107281.00046419843 grad=13987536.012562865, beta=
0.0
iteration 789 bound=-105177.5375011299 grad=8588580.630748732, beta=0.0
iteration 791 bound=-110790.75730606032 grad=942742.1252450955, beta=0.
0
iteration 792 bound=-105519.37028499918 grad=20895414.11372856, beta=0.
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iteration 794 bound=-106040.00872511654 grad=3673975.9028284904, beta=
0.0
iteration 796 bound=-108327.27090142506 grad=5553724.103775831, beta=0.
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iteration 797 bound=-105198.73797537136 grad=13060360.815248478, beta=
0.0
iteration 799 bound=-109450.18044735231 grad=1339580.4012452557, beta=
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iteration 800 bound=-105636.02491323774 grad=8320567.354972067, beta=0.
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iteration 802 bound=-111388.48677338658 grad=2067213.3727782597, beta=
0.0
iteration 803 bound=-109865.7925447831 grad=21741896.245409895, beta=0.
0
iteration 804 bound=-105447.44079404145 grad=15079070.586502362, beta=
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iteration 806 bound=-110895.44110181155 grad=572148.704953063, beta=0.0
iteration 807 bound=-107356.64412762689 grad=3703232.1056921687, beta=
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iteration 809 bound=-111809.20559504633 grad=12226776.50783065, beta=0.
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iteration 810 bound=-108037.32359820174 grad=10671293.747428877, beta=
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iteration 811 bound=-106462.44139759992 grad=14225085.792202896, beta=
0.0
iteration 813 bound=-111706.21947396666 grad=9601540.900011586, beta=0.
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iteration 814 bound=-105406.0016478035 grad=820554.4406527588, beta=0.0
iteration 816 bound=-109513.01635083131 grad=1282636.3296963046, beta=
0.0
```

```
iteration 817 bound=-105812.55914503765 grad=11116488.531597646, beta=
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iteration 819 bound=-110773.5742681318 grad=1100954.1557694932, beta=0.
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iteration 821 bound=-114581.6353019685 grad=22693064.037942845, beta=0.
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iteration 822 bound=-106798.34393892714 grad=11358579.909066165, beta=
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iteration 824 bound=-108006.69698498212 grad=9350714.94942683, beta=0.0
iteration 825 bound=-105343.19851687372 grad=11729711.96235011, beta=0.
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iteration 827 bound=-105771.8163491905 grad=1324892.0777754148, beta=0.
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iteration 829 bound=-114164.13209741701 grad=307207.8727406104, beta=0.
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iteration 830 bound=-105693.75830073589 grad=12022710.041868601, beta=
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iteration 832 bound=-105718.34851015937 grad=4166057.4536168864, beta=
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iteration 835 bound=-105675.67462250064 grad=12287422.381561816, beta=
0.0
iteration 837 bound=-111546.25134757897 grad=963221.3699796535, beta=0.
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iteration 839 bound=-112228.07314102727 grad=525174.722598398, beta=0.0
iteration 840 bound=-105533.86555925274 grad=4455717.017298222, beta=0.
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iteration 841 bound=-105077.23419836782 grad=937663.0259762517, beta=0.
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iteration 843 bound=-110639.57221446717 grad=442740.4486160327, beta=0.
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iteration 845 bound=-122795.00875585974 grad=23856964.06761978, beta=0.
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iteration 846 bound=-106314.28041039596 grad=23058987.213692002, beta=
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iteration 848 bound=-112695.60242007033 grad=7394993.35952279, beta=0.0
iteration 849 bound=-105456.63101823164 grad=1093837.0228072994, beta=
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iteration 850 bound=-105341.53577228292 grad=414950.79063871177, beta=
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iteration 852 bound=-109026.34882545595 grad=739280.7195352146, beta=0.
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iteration 853 bound=-106727.00090596204 grad=12871764.107393414, beta=
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iteration 855 bound=-112429.278911316 grad=8664757.032281313, beta=0.0
iteration 857 bound=-113835.49944539742 grad=16062365.078121688, beta=
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iteration 858 bound=-111464.13726621679 grad=7994938.313934743, beta=0.
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0
iteration 860 bound=-105436.52735735796 grad=11282764.678171726, beta=
0.0
iteration 862 bound=-105730.9580019404 grad=759758.9580558429, beta=0.0
iteration 864 bound=-113103.12017164232 grad=522495.40148823103, beta=
0.0
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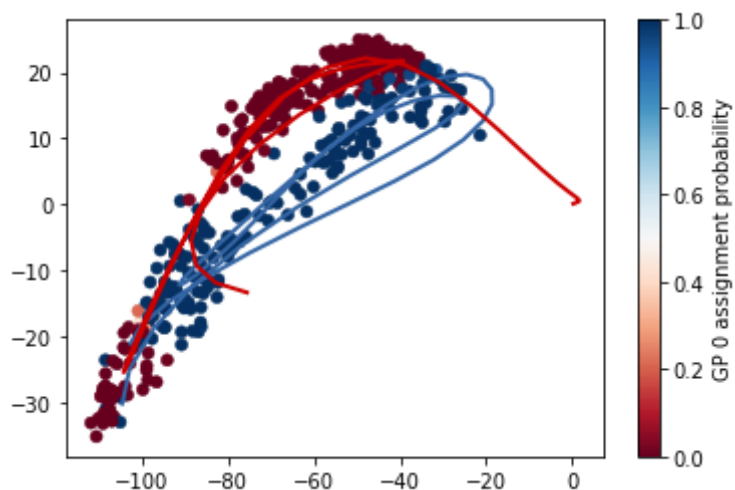
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iteration 866 bound=-124643.82101597938 grad=1579466.3585878655, beta=
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iteration 867 bound=-111360.79850418825 grad=9179041.657945575, beta=0.
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iteration 868 bound=-106540.96590277426 grad=14417735.976576697, beta=
0.0
iteration 869 bound=-105180.0666717162 grad=6130715.155511389, beta=0.0
iteration 871 bound=-105446.09061134863 grad=1051456.9800670391, beta=
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iteration 873 bound=-118282.8646657124 grad=950574.0502087635, beta=0.0
iteration 874 bound=-107171.68547111787 grad=9580688.210454572, beta=0.
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iteration 876 bound=-109512.65996633346 grad=9769026.38019711, beta=0.0
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iteration 879 bound=-105383.61615297092 grad=757541.2744816178, beta=0.
0
iteration 881 bound=-111730.03620729232 grad=679225.3338791541, beta=0.
0
iteration 883 bound=-117832.97896014074 grad=1196686.7697104986, beta=
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iteration 884 bound=-105332.05841944311 grad=26799026.060098737, beta=
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iteration 886 bound=-106055.25777719993 grad=237825.09409917024, beta=
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iteration 887 bound=-105443.31087477467 grad=2210419.430890468, beta=0.
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iteration 890 bound=-106713.44564120108 grad=9457241.276894057, beta=0.
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iteration 891 bound=-105719.65176988159 grad=9056117.418754542, beta=0.
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iteration 892 bound=-105639.98869810428 grad=2117283.4398087226, beta=
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iteration 894 bound=-106119.00804264603 grad=523979.51834665466, beta=
0.0
iteration 896 bound=-111921.21175545089 grad=4918084.49012257, beta=0.0
iteration 897 bound=-105247.18442419815 grad=2660267.9274481903, beta=
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iteration 899 bound=-109206.21174038209 grad=758745.9464597695, beta=0.
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iteration 900 bound=-105599.05544718813 grad=11234332.209709352, beta=
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iteration 902 bound=-113471.74256729416 grad=573635.2655048021, beta=0.
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iteration 903 bound=-111716.10198189577 grad=9422933.207073914, beta=0.
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iteration 904 bound=-111075.31804711933 grad=2227427.675018996, beta=0.
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iteration 905 bound=-105781.05609386048 grad=25560302.89724682, beta=0.
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iteration 906 bound=-105274.8975697762 grad=1588175.27437546, beta=0.0
iteration 908 bound=-110860.27150963478 grad=1144546.6215352083, beta=
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iteration 911 bound=-105453.33834203199 grad=21059101.524993386, beta=
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0.0
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iteration 915 bound=-105275.34163068175 grad=13848412.617724596, beta=
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iteration 929 bound=-113944.68448340103 grad=223464.8273648889, beta=0.
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iteration 937 bound=-107766.03274753549 grad=5305971.741654343, beta=0.
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iteration 939 bound=-116912.83149096734 grad=12532967.554408308, beta=
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iteration 940 bound=-105707.5167450474 grad=26616022.247751903, beta=0.
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iteration 941 bound=-105424.80115078375 grad=2455570.616152561, beta=0.
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iteration 943 bound=-105560.61705543016 grad=556421.924060163, beta=0.0
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iteration 946 bound=-105517.85586531452 grad=19755410.507296998, beta=
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iteration 948 bound=-118054.25764482743 grad=1618133.5444774628, beta=
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iteration 949 bound=-107110.48621626875 grad=5073257.5853702305, beta=
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iteration 951 bound=-112894.17672522638 grad=9821669.689427495, beta=0.
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iteration 952 bound=-105379.15666631873 grad=2497397.356651902, beta=0.
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iteration 954 bound=-106086.13282808922 grad=1592150.773784549, beta=0.
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iteration 956 bound=-107893.02089280038 grad=3299065.7491533495, beta=
```

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0.0
iteration 958 bound=-109446.86862038847 grad=13575222.616481224, beta=
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iteration 959 bound=-106178.86616181425 grad=17141173.23240149, beta=0.
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iteration 960 bound=-106088.51607253044 grad=3561405.3312572017, beta=
0.0
iteration 962 bound=-116281.11449887347 grad=6046639.748550413, beta=0.
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iteration 963 bound=-105501.30987211256 grad=14394816.487365404, beta=
0.0
iteration 965 bound=-107654.25557680811 grad=1000854.8970380186, beta=
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iteration 966 bound=-107401.73711270654 grad=9862173.02912684, beta=0.0
iteration 967 bound=-105171.77142336706 grad=11891522.141364684, beta=
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iteration 973 bound=-115995.41006616202 grad=3168586.01576926, beta=0.0
iteration 974 bound=-105602.28041012013 grad=14813855.498853989, beta=
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iteration 975 bound=-105498.73025953061 grad=2517921.894835502, beta=0.
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iteration 983 bound=-107111.61646259027 grad=3490922.0996142463, beta=
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iteration 985 bound=-120423.43585010781 grad=10636732.997237753, beta=
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0.0
maxiter exceeded
```



```
/scratch/groups/abattle4/josh/gp_fates/GPfates/GPfates.py:91: FutureWarning: Method .as_matrix will be removed in a future version. Use .values instead.
```



Looks like PCA doesn't cut it here. However, since they do pseudotime inference first and bifurcation analysis later, in theory a different pseudotime metric would work okay