GP_model_checking_test_cases_rjf

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1 Gaussian process model checking: test cases

Here we test model checking diagnostics patterned after Bastos-O'Hagan:

```
Leonardo S. Bastos and Anthony O'Hagan,
<a href="https://doi.org/10.1198/TECH.2009.08019"> <i>Diagnostics for Gaussian Process Emulators
Technometrics <b>51</b>, 425 (2009).
```

The diagnostic functions are from the gsum module written by Jordan Melendez.

Last revised 10-Dec-2018 by Dick Furnstahl [furnstahl.1@osu.edu], building on the original notebook by Jordan Melendez and modifications by Daniel Phillips.

1.1 Overview of B&O Model Checking Implementation

Bastos & O'Hagan provide a versatile set of diagnostic tools for testing whether or not a Gaussian process (GP) is a reasonable emulator for an expensive simulator. Our use case is slightly different than theirs. We don't necessarily care about our GPs matching some underlying simulator. Rather, given a set of curves from a hierarchy of simulators, we wish to answer the following questions: 1. Can they reasonably be assumed to be drawn from the same underlying Gaussian process? 2. If so, which Gaussian process? 3. The underlying GP is later used as a model discrepancy, so how can we test its performance against experiment?

These three questions may or may not be decided by diagnostics discussed in B&O, but to find out we must implement their methods! This notebook tests our adaptations of their methods.

1.2 Modules to import

(rjf note: imports in the original notebook that were moved to gsum have been removed.)

```
In [1]: # standard python: see online documentation
        import numpy as np
        import scipy as sp

        # For plotting we use matplotlib; other choices are possible
        import matplotlib as mpl
        import matplotlib.pyplot as plt

        # special imports for python programming: see online documentation
        from itertools import cycle

        # scikit-learn machine learning  https://scikit-learn.org/stable/modules/classes.html
        from sklearn.gaussian_process import GaussianProcessRegressor
           # see https://scikit-learn.org/stable/modules/gaussian_process.html
           #  for documentation. Main excerpt:
           # The GaussianProcessRegressor implements Gaussian processes (GP) for
           #  regression purposes. For this, the prior of the GP needs to be specified.
           #  The prior mean is assumed to be constant and zero (for normalize_y=False)
           #  or the training datas mean (for normalize_y=True).
           #  The priors covariance is specified by passing a kernel object.
           #  The hyperparameters of the kernel are optimized during fitting of
           #  GaussianProcessRegressor by maximizing the log-marginal-likelihood (LML)
           #  based on the passed optimizer. If the initial hyperparameters should be kept
           #  fixed, None can be passed as optimizer.
        from sklearn.gaussian_process.kernels import RBF, ConstantKernel as C, WhiteKernel
           # RBF is a particular GP kernel (radial-basis function kernel, aka
           #  squared-exponential kernel).
           # ConstantKernel: "Can be used as part of a product-kernel where it scales the
           #  magnitude of the other factor (kernel) or as part of a sum-kernel, where it
           #  modifies the mean of the Gaussian process."
           # WhiteKernel: "The main use-case of this kernel is as part of a sum-kernel where
           #  it explains the noise-component of the signal. Tuning its parameter corresponds
           #  to estimating the noise-level."

        # gsum is the package written by Jordan Melendez
        import gsum
        from gsum import rbf, default_attributes, cholesky_errors, mahalanobis
        from gsum import lazy_property, pivoted_cholesky
        from gsum import ConjugateGaussianProcess, ConjugateStudentProcess
        from gsum import Diagnostic, GraphicalDiagnostic
```

```
In [2]: # set rcParams here
        mpl.rcParams['figure.dpi'] = 120
```

```
In [3]: %matplotlib inline
```

1.3 Test case

This test case will generate toy data from the same given GP by sampling a few curves and selecting a set of training points from each curve. Then we fit a GP to the data.

1.3.1 Parameters to adjust

```
In [4]: output_directory = './saved_notebooks'
        output_filename = 'DP_model_breaking_2_big_scale_shift'

        # mesh points for the GPs (x_num points from x_min to x_max)
        x_min = 0
```

```
x_max = 20
x_num = 41
X_full = np.atleast_2d(np.linspace(x_min, x_max, x_num)).T

# toy data points (every data_skip points starting with data_offset point)
data_skip = 5
data_offset = 0   # should be less than data_skip
from math import ceil
data_pts = ceil(x_num/data_skip)
# mask array True entry if corresponding point is in training data, otherwise False
mask = np.array([(i-data_offset) % data_skip == 0 for i in range(len(X_full))])

n_samples = 3  # draw n_samples curves
n_ref = 1000   # number of diagnostic samples (should this ever change?)

# DP characterization of the GP(s) used to sample the toy data.
#  Specifies hyperparameters (hps) var and length scale for each GP
basevar = 1.0; varshiftfactor=1; baselengthscale=3; lengthscaleshift=1;
#basevar = 1.0; varshiftfactor=2; baselengthscale=3; lengthscaleshift=0;
#basevar = 1.0; varshiftfactor = 1.0; baselengthscale = 3; lengthscaleshift = 0;
toy_gp_hps = [ [basevar, baselengthscale],
               [basevar*varshiftfactor, baselengthscale+lengthscaleshift],
               [basevar/varshiftfactor, baselengthscale-lengthscaleshift] ]
# More generally, use toy_gp_hps = [ [var0, ls0], [var1, ls1], ...]

seed = 2
toy_gp_seeds = seed + np.arange(n_samples)  # array of n_samples values
# Here specified as ascending integers starting from an initial seed,
#  but they could be specified by hand or randomized

nugget_sd = 1e-4  # Check if we are sensitive to the value

# Vertical lines (True) or a histogram (False) for the md and kl plots
vlines = True
```

Print a table with specs for the samples:

```
In [5]: gps_cycle = cycle(np.arange(len(toy_gp_hps)))   # go through gps cyclically
        print('sample #   variance  length scale  color')
        for i in range(n_samples):
            gp_index = next(gps_cycle)
            print('   {0:d}          {1:.2f}        {2:.1f}   '\
                  .format(i, toy_gp_hps[gp_index][0], toy_gp_hps[gp_index][1]))
```

```
sample #   variance  length scale  color
   0          1.00        3.0
   1          1.00        4.0
   2          1.00        2.0
```

1.3.2 Ok, let's roll!

```
In [6]: # Set up array of kernels and gps
        # Each kernel is the sum of an RBF kernel scaled by the variance and a noise kernel
        toy_gp_kernel = []
        toy_gp = []
        for i in range(len(toy_gp_hps)):
            toy_gp_kernel.append( C(toy_gp_hps[i][0], (1e-3, 1e3)) \
                                    * RBF(toy_gp_hps[i][1], (1e-2, 1e2)) \
                                  + WhiteKernel(nugget_sd**2) )
            toy_gp.append( GaussianProcessRegressor(kernel=toy_gp_kernel[i], optimizer=None) )

        # kernel with starting hyperparameters
        base_gp_kernel = C(basevar, (1e-3, 1e3)) * RBF(baselengthscale, (1e-2, 1e2))
```

Generate full toy data and split into training and test data.

```
In [7]: # Sample the gps at all of the X points
        toy_data_full = []      # toy data at X_full
        toy_data_training = []  # the points used to train
        toy_data_test = []      # the remaining points
        gps_cycle = cycle(np.arange(len(toy_gp_hps)))   # sample from gps cyclically
        for i in range(n_samples):
            toy_data_full.append( toy_gp[next(gps_cycle)].sample_y(X_full, n_samples=1,
                                                            random_state=toy_gp_seeds[i]).T )
            toy_data_training.append( toy_data_full[i][:, mask] )
            toy_data_test.append( toy_data_full[i][:, ~mask])
        toy_data_full = np.concatenate(toy_data_full)
        toy_data_training = np.concatenate(toy_data_training)
        toy_data_test = np.concatenate(toy_data_test)

        X_training = X_full[mask]
        X_test = X_full[~mask]
```

Now we fit the data and compute means and covariances:

```
In [8]: my_gp = ConjugateGaussianProcess(base_gp_kernel)
        my_gp.fit(X_training, toy_data_training)

        # compute the mean and covariance of the fitted GP at the training set points
        fitmean = my_gp.mean(X_training)
        fitcov = my_gp.cov(X_training)

        # compute the values of the fitted GP at all the data points
        X_pred = X_full  # should switch to X_test
        m_pred, K_pred = my_gp.predict(X_pred, return_cov=True, pred_noise=True)
        # print(np.diag(K_pred))
        sd_pred = np.sqrt(np.diag(K_pred))
```

```
# compute the mean and covariance of the overall GP at the set X_full
fitmean_full = my_gp.mean(X_pred)
fitcov_full = my_gp.cov(X_pred,X_pred)
```

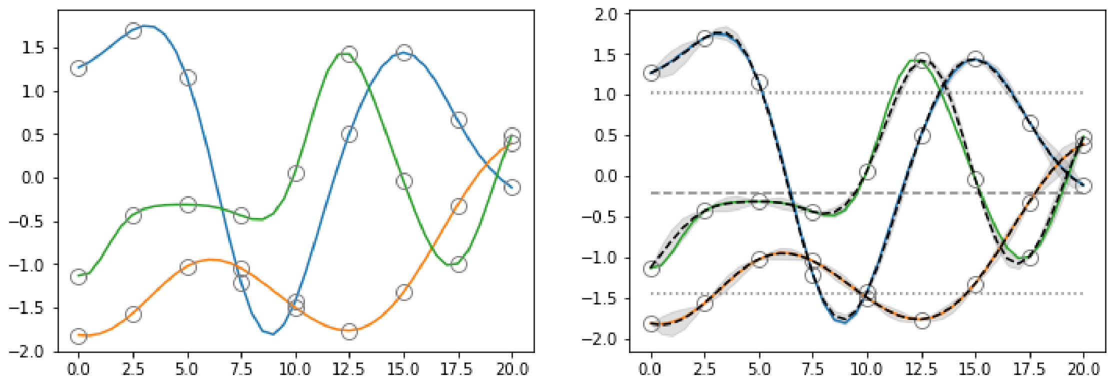
1.3.3 Plot the toy data and fits

```
In [9]: # Plot the gps, test data, and fits
        fig = plt.figure(figsize=(12,4))
        ax1 = fig.add_subplot(1,2,1)
        ax1.plot(X_full.ravel(), toy_data_full.T);
        ax1.plot(X_training.ravel(), toy_data_training.T,
                 ls='', marker='o', fillstyle='none', markersize=10, c='gray');


        ax2 = fig.add_subplot(1,2,2)
        # Plot the underlying process
        ax2.plot(X_training.ravel(), my_gp.mean(), ls='--', c='gray')
        ax2.plot(X_training.ravel(), my_gp.mean() + my_gp.sd(), ls=':', c='gray')
        ax2.plot(X_training.ravel(), my_gp.mean() - my_gp.sd(), ls=':', c='gray');

        # Now the true data
        ax2.plot(X_full.ravel(), toy_data_full.T);
        ax2.plot(X_training.ravel(), toy_data_training.T, ls='', marker='o',
                 fillstyle='none', markersize=10, c='gray');

        # The predicted interpolants and their errors
        ax2.plot(X_pred.ravel(), m_pred.T, c='k', ls='--', label='pred');
        for m in m_pred:
            ax2.fill_between(X_pred.ravel(), m + 2*sd_pred, m - 2*sd_pred,
                             color='gray', alpha=0.25)
        # ax2.legend();
```



Comments:

[dp] It worked: blue curve is the original length scale (3), orange has a larger length scale (4), and green a smaller one (2). Orange is "lazy" and green is "too active". Interpolant for green

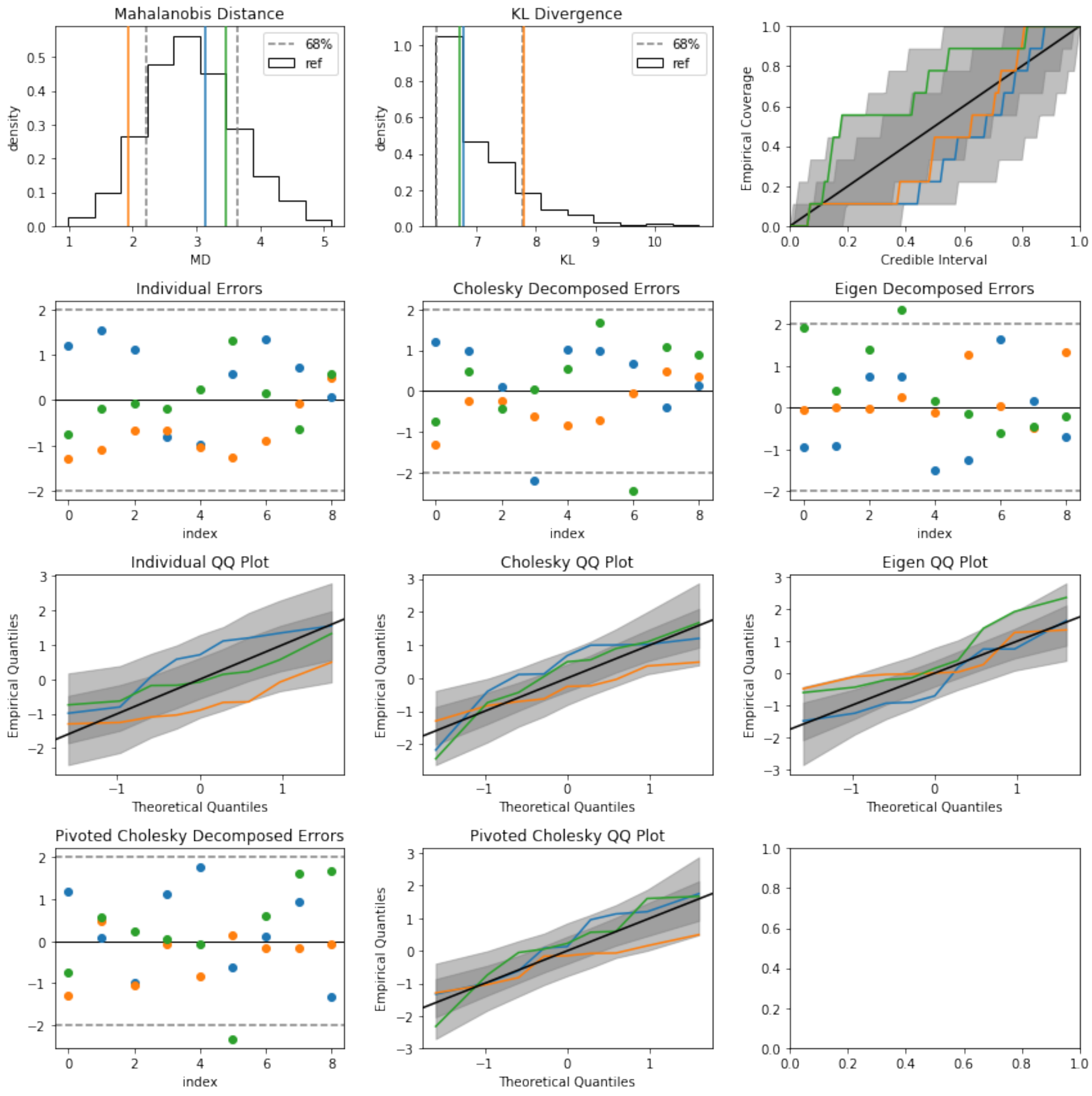
curve is in a spot of bother. And note that the GP has increased the variance a bit in order to accommodate the disparate length scales.

[rjf] Same figures as dp.

We can do better than these "by eye" checks. What does B&O model checking say about this case? First, assume that we are checking the underlying process, shown by the constant gray dotted/dashed lines above, against the colored draws.

1.3.4 Use the training data only

```
In [10]: np.random.seed(seed)
         gp = ConjugateGaussianProcess(base_gp_kernel)
         gpmc = Diagnostic(fitmean, fitcov)
         gd = GraphicalDiagnostic(gpmc, toy_data_training, nref=n_ref)
         gd.plotzilla(X_training, gp, vlines=vlines);
```



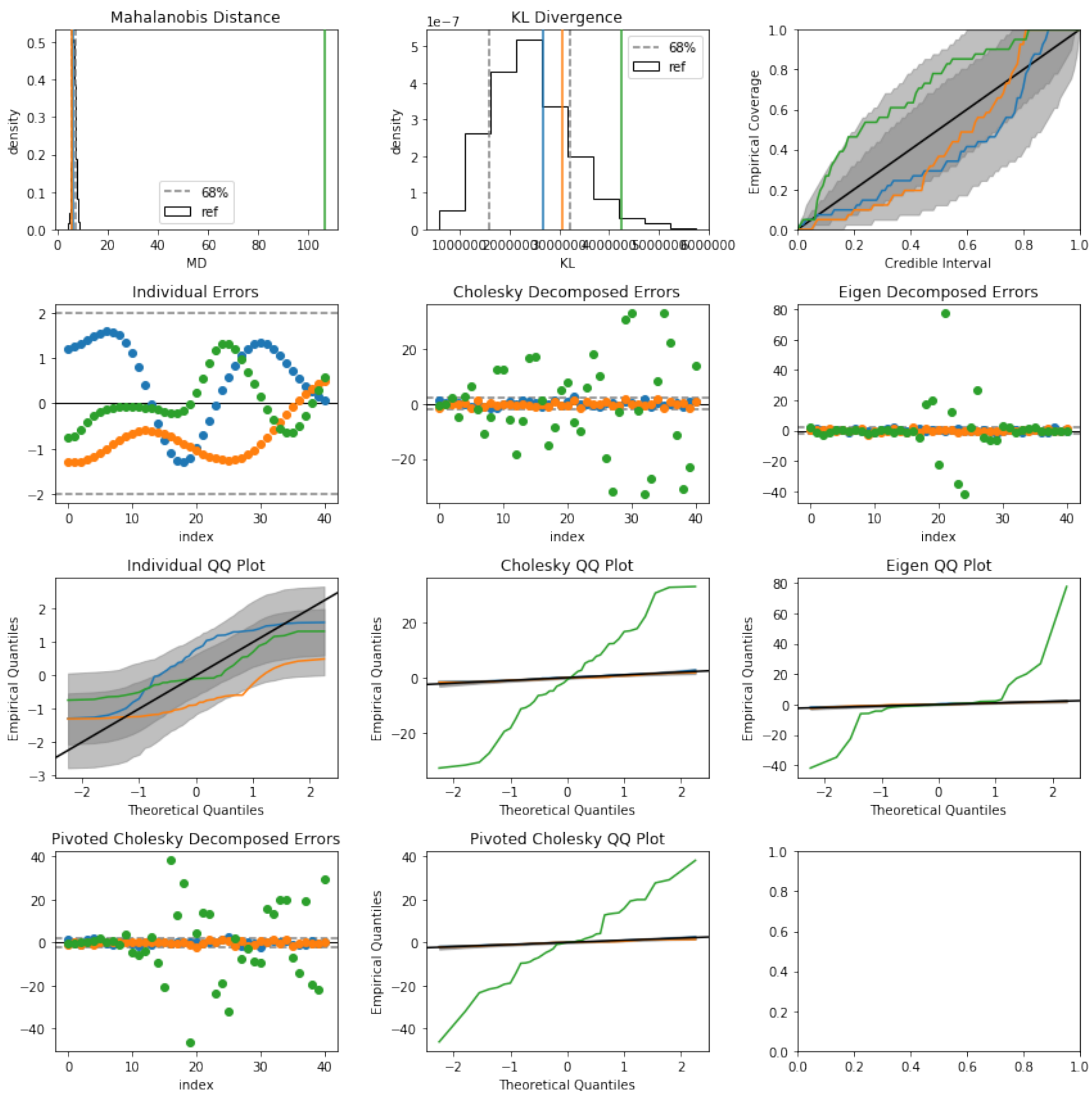
Comments:

[dp] Nothing too dramatic here, although if one is being paranoid one would worry about the lack of 2-sigma outliers in the orange set.

1.3.5 Use the full dataset

```
In [11]: # At the moment we do this test against the full data set, although we may decide
         #  to remove training data later
         toy_data_pred = toy_data_full
```

```
In [12]: gp = ConjugateGaussianProcess(base_gp_kernel)
         gpmc_full = Diagnostic(fitmean_full,
                                fitcov_full + nugget_sd**2 * np.eye(fitcov_full.shape[0]))
         gd_full = GraphicalDiagnostic(gpmc_full, toy_data_pred, nref=n_ref)
         gd_full.plotzilla(X_full, gp, vlines=vlines);
```



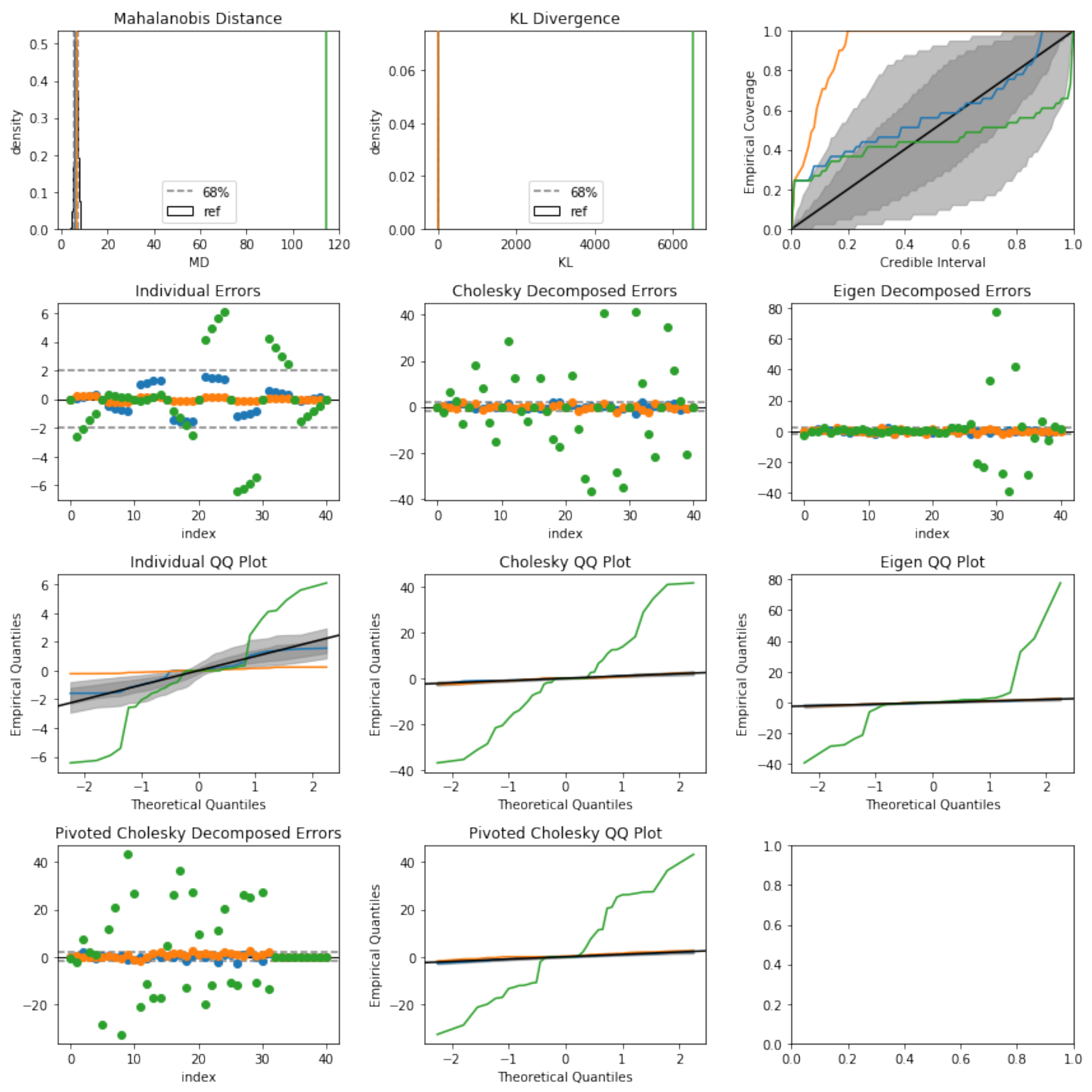
Comments:

[dp] Now the proverbial spaghetti hits the fan. MD for green curve is massive. Note that its the PC errors at larg(ish) index (and/or eigen-errors at intermediate index) that are responsible for generating this large MD. QQ plot also massively screwed up. But note that failure in DCI plot is not as dramatic.

1.3.6 Model checking with the interpolants

What if we performed the same model checking with the interpolants? This time, we are comparing each colored curve to the process defined by the thin gray bands around that curve. One potential clever way to combine the diagnostics from interpolated processes relies on the fact that the only thing that is different about the interpolating processes is their mean function that interpolates the data. If we subtract the means off the process and the data, then we are back to the simple iid case.

```
In [13]: np.random.seed(seed)
         gp = ConjugateGaussianProcess(base_gp_kernel, v0=0)
         gp.fit(X_training, toy_data_training, noise_sd=nugget_sd)
         mean_est, cov_est = gp.predict(X_pred, return_cov=True, pred_noise=True)
         # print(mean_est.shape)
         gpmc = Diagnostic(np.zeros(m_pred.shape[1]), K_pred \
                           + nugget_sd**2 * np.eye(K_pred.shape[0]))
         # gpmc = GPModelChecking(np.zeros_like(mean_est[0]), cov_est, df=2*gp.a())
         gd = GraphicalDiagnostic(gpmc, toy_data_pred - m_pred, nref=n_ref)
         gd.plotzilla(X_pred, gp, predict=True, vlines=vlines);
```



Comments:

[dp] I do not understand why the large PC decomposed errors show up here at intermediate index. Is that because the training points define a set of high-index small errors? So if we separated off the training & testing data the problem would again be at large index?

```
In [14]: # *** RUN THIS CELL AFTER YOU HAVE SAVED THE NOTEBOOK ***
         # save as a pdf file
         !jupyter nbconvert GP_model_checking_test_cases_rjf.ipynb --to pdf \
                            --output-dir=$output_directory --output $output_filename \
                            >/dev/null 2>&1
```