Gaussian Process: Causal, Anticausal, Bilateral components [Matlab example]

*Executed in Matlab **R2023b**

Presentations in video:

http://personales.upv.es/asala/YT/V/gpcholEN.html

http://personales.upv.es/asala/YT/V/gpanticaEN.html

Objectives: A Gaussian Process is a "random function". Let us look at the "latent" variables from which the GP can be generated based on the different possibilities of matrix square roots of the covariance matrix.

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Prior mean and covariance kernel

```
Data.X=[]; Data.Y=[]; %To test "prior" model
Data.K=@K;
Xtest=-3:(1/30):5; %uniform grid to test stuff, dense enough...
LL=length(Xtest)
```

```
LL = 241
```

```
PredPrior=zeros(3,LL); %we'll predict confidence interval and mean
[Mean,CovMatrix]=predictGP(Xtest,Data);
```

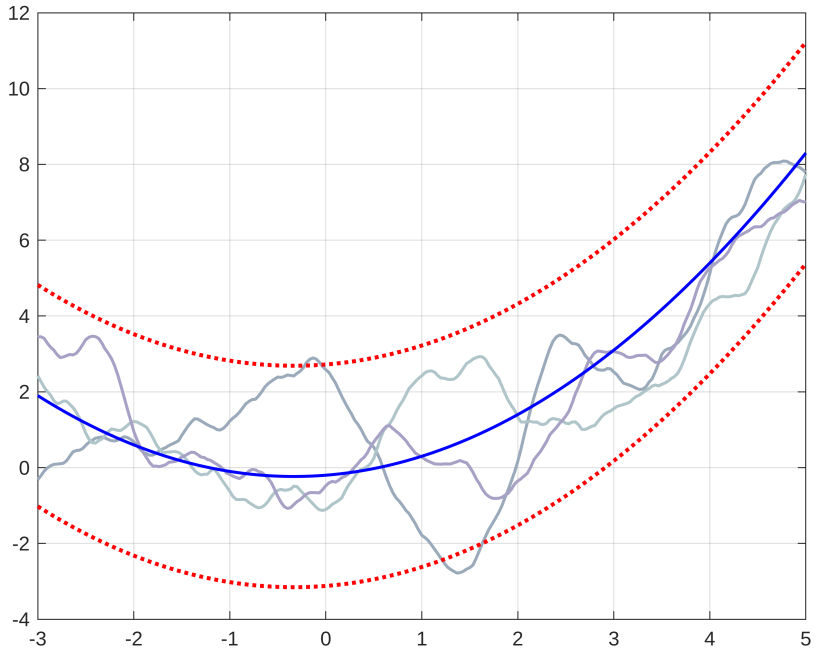
The prior is stationary (given how we defined it at the end of the file).

Confidence bounds and example samples

```
sg=sqrt(diag(CovMatrix)); %std. dev.
PredPrior=[Mean+1.96*sg Mean Mean-1.96*sg];
NTrials=3;
```

```
F1=mvnrnd(Mean,CovMatrix+1e-10*eye(LL),NTrials);

for i=1:NTrials
    if(NTrials<4)
        LW=1.5;
    else
        LW=1;
    end
    col=[.4 .55 .7]+rand()*[.3 0 0]+rand()*[0 .25 0]+rand()*[0 0 0.2];
    plot(Xtest,F1(i,:),Color=col,LineWidth=LW), hold on
end
plot(Xtest,PredPrior(:,2),'b',LineWidth=1.5), grid on
plot(Xtest,PredPrior(:,[1 3]),':r',LineWidth=2), hold off
```



Square root of covariance matrix (discretized at test points), interpretation

If we have samples of the GP, call them y_k, $1 \le k \le 241$ in our case, and the covariance matrix $K_{241\times241}$ can be factorised as $K = Q_{241\times241} \cdot Q^T_{241\times241}$, we'll say that Q is a "matrix" square root of K.

So, the GP (well, increments from its mean function) can be generated by "latent" standard normal random variables ξ, as $y = Q\xi_{241\times1}$, $\xi \sim N(0, I_{241})$ because, indeed, the covariance matrix is $E[yy^T] = E[Q\xi\xi^TQ^T] = Q \cdot E[\xi\xi^T] \cdot Q^T = Q \cdot I \cdot Q^T = K$. The internals of Matlab's `mvnrnd` work based on this fact.

*Other authors may say that B is a square root of a if $B \cdot B = A$, so be aware on which definition is used if you look up elsewhere. In here, we will use the $A = B \cdot B^T$ interpretation, only valid for symmetric matrices, of course.

Matrix square root is not unique, as any orthogonal matrix U, i.e., fulfilling $UU^T = I$ generates another square root QU because $K = (QU) \cdot (U^T Q^T)$.

Different matrix square roots have different interpretations of the "latent" random variables.

There will be several of them with interest in discrete-time stochastic processes: the "orthogonal" (diagonalisation, Karhunen-Loeve), the "triangular" (Cholesly, causal or anticausal representations) and the "symmetric" one, to be discussed in several videos in the collection.

Of course, there is theory generalising to the "discrete-time" going from $-\infty$ to $+\infty$ and to the full "continuous-time" case (spectral factor, all-pass functions, Fourier features) but it is more involved, out of the scope here...

Diagonalization of covariance matrix (discretized at test points), orthogonal square root

Further detail in previous video.

```
[V,D]=eig(CovMatrix); %eigenvalues + eigenvectors
[eevv,idx]=sort(diag(D),1,"descend");
V=V(:,idx); D=D(:,idx); %we sort eigenvalues and eigenvectors to match
minev=min(eevv); %eevv are positive... except for numerical tolerance
issues...
eevv=eevv+max(0,-minev); %now minimum is non-negative
```

Note: we carried out principal component analysis (meaning of eigenvalues and eigenvectors of covariance matrix)... If we have "many" points, we do approach the continuous GP eigenfunctions and eigenvalues, the Karhunen-Loeve ones:

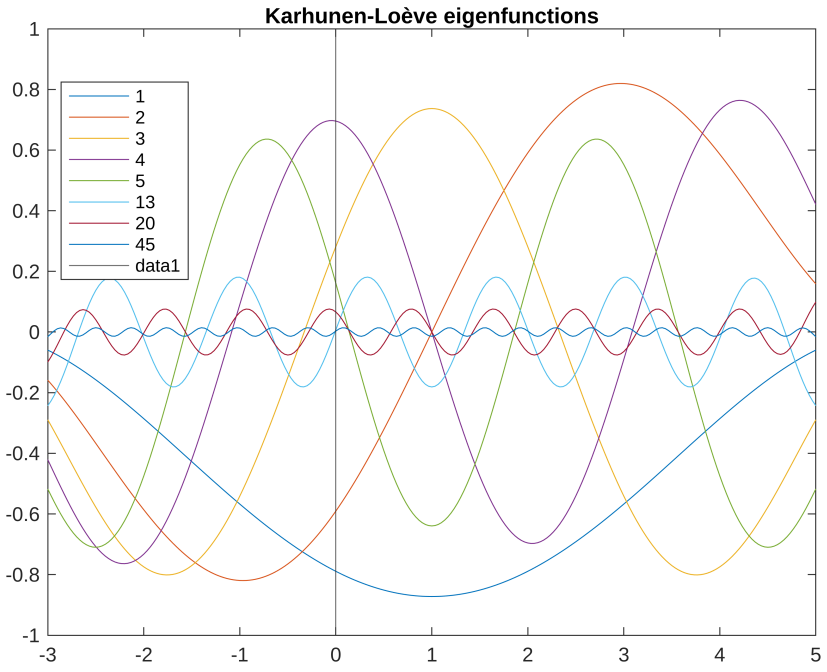
$Kv_i = \lambda_i v_i$ (matrix eigenvectors) get converted in the limit case to $\Rightarrow \quad \int_{-2}^{2} \kappa(x,s) \cdot \phi_i(s)\, ds = \lambda_i \cdot \phi_i(x)$

covariance kernel eigenfunctions

Let us have a look at the eigenvectors (i.e., eigenfunctions):

```
PrincCom=V*diag(sqrt(abs(eevv)));
plot(Xtest,PrincCom(:,[1 2 3 4 5 13 20 45])),
legend("1","2","3","4","5","13","20","45", Location="best")
xline(0)
```

```
title("Karhunen-Loève eigenfunctions")
```




```
Q=PrincCom; %matrix square root for animation
%return
```

*Execute animPCA.m script now.

Cholesky square root factorization (triangular) of covariance matrix, CONVOLUTION representation

Let us now discuss the "lower triangular" square root.

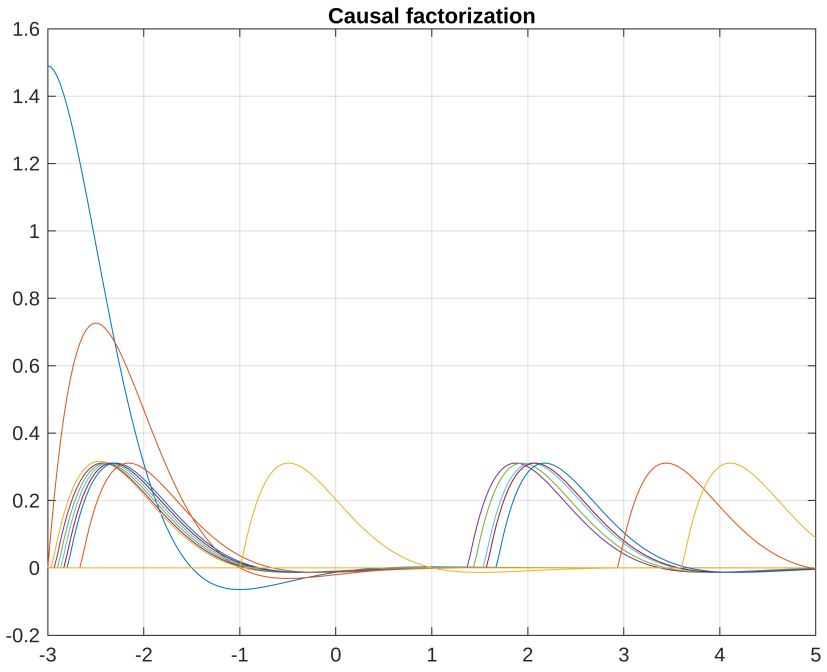
```
Q=chol(CovMatrix+1e-15*eye(LL),'lower');
Q
```

```
Q = 241×241
    1.4905         0         0         0         0         0         0         0 ···
    1.4865    0.1084         0         0         0         0         0         0
    1.4752    0.2090    0.0390         0         0         0         0         0
    1.4574    0.2985    0.0837    0.0379         0         0         0         0
    1.4337    0.3776    0.1236    0.0819    0.0378         0         0         0
    1.4049    0.4468    0.1588    0.1212    0.0818    0.0378         0         0
    1.3717    0.5068    0.1898    0.1559    0.1210    0.0818    0.0378         0
    1.3346    0.5582    0.2166    0.1863    0.1557    0.1210    0.0818    0.0378
    1.2943    0.6016    0.2397    0.2128    0.1861    0.1557    0.1210    0.0818
    1.2512    0.6375    0.2592    0.2355    0.2125    0.1861    0.1557    0.1210
     ⋮
```

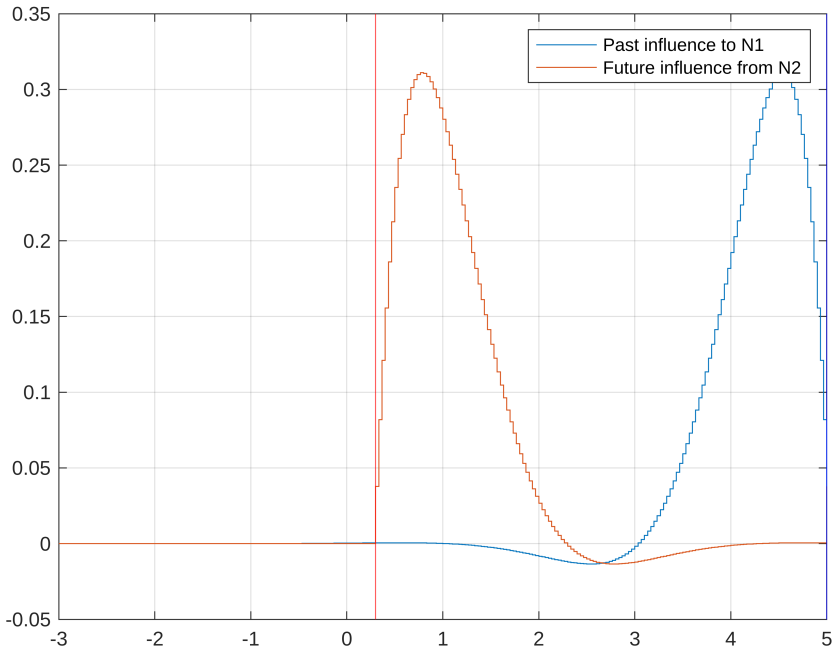
```
norm(Q*Q'-CovMatrix) %it is indeed a matrix square root
```

```
ans = 7.3271e-15
```

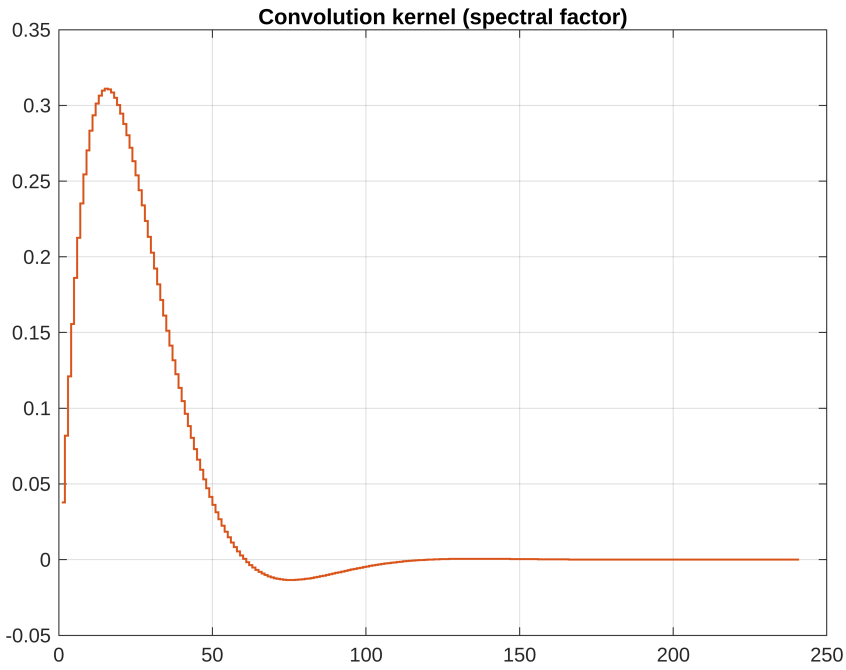
```
plot(Xtest,Q(:,[1 2 3 4 5 6 7 8 12 62 133 135 138 139 142 180 200])), grid on
title("Causal factorization")
```




```
N1=241;
stairs(Xtest,Q(N1,:)), grid on
hold on
N2=100;
stairs(Xtest,Q(:,N2)), hold off, xline(Xtest(N2),'r'), xline(Xtest(N1),'b')
legend("Past influence to N1", "Future influence from N2")
```




```
stairs(Q((N2):end,N2),LineWidth=1), hold on,
stairs(fliplr(Q(N1,:)),LineWidth=1), hold off, grid on, title("Convolution
kernel (spectral factor)")
```



Triangular structure: the GP can be expressed by the formula

$$y_k = \sum_{j \le k} q_{kj} \xi_j$$

because, if it is lower triangular $q_{ij} = 0$ for $j > k$, so no need to appear in the matrix product expression.

And, well, except for the first samples, columns are the same as rows.

If the nonzero elements of a column are denoted as the sequence $\{h_0, h_1, \dots\}$ then, when initial condition (or "finite window processing") effects have vanished (we need to close a column "far away from the left"), the row is the column "flipped", and the response is:

$$y_k = \sum_{j \le k} h_{k-j} \xi_j$$

which is called the "convolution formula... only truly valid at least in formal discussion if "past" extends indefinitely so sum is from $j = -\infty$ so indeed there is no effect of initial conditions or "finite window" signal processing. Of course, the idea can be extended to continuous-time convolution kernel $y(t) = \int_{-\infty}^{t} h(t-s)\xi(s)\, ds$, with formal difficulties as $\xi(s)$ is a white-noise with infinite variance, etc. (out of the scope of this material).

Execute **`animChol.m`** NOW.

```
```

Let's see the anticausal option: correlation does not imply causality and everything can be "repeated" if we consider right-to-left progression of random variables.

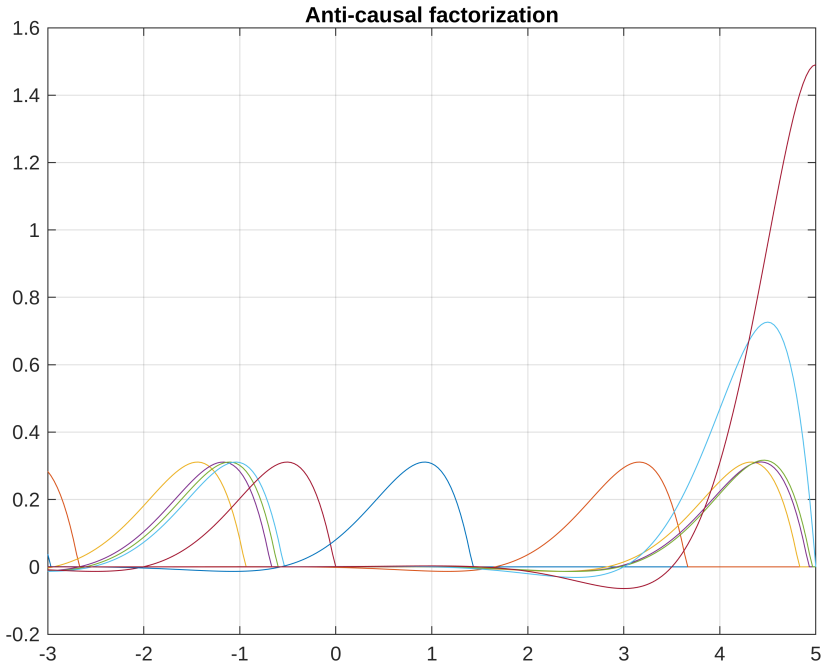
```
Qflip=fliplr(flipud(Q))
```

```
Qflip = 241×241
    0.0378    0.0818    0.1210    0.1557    0.1861    0.2125    0.2352    0.2544 ···
         0    0.0378    0.0818    0.1210    0.1557    0.1861    0.2125    0.2352
         0         0    0.0378    0.0818    0.1210    0.1557    0.1861    0.2125
         0         0         0    0.0378    0.0818    0.1210    0.1557    0.1861
         0         0         0         0    0.0378    0.0818    0.1210    0.1557
         0         0         0         0         0    0.0378    0.0818    0.1210
         0         0         0         0         0         0    0.0378    0.0818
         0         0         0         0         0         0         0    0.0378
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
    ⋮
```

```
norm(Qflip*Qflip'-CovMatrix)
```

```
ans = 2.2911e-14
```

```
plot(Xtest,Qflip(:,[1 10 62 70 72 74 90 133 200 235 238 239 240 241])), grid
on
title("Anti-causal factorization")
```




```
Q=Qflip;% for animation
```

```

```

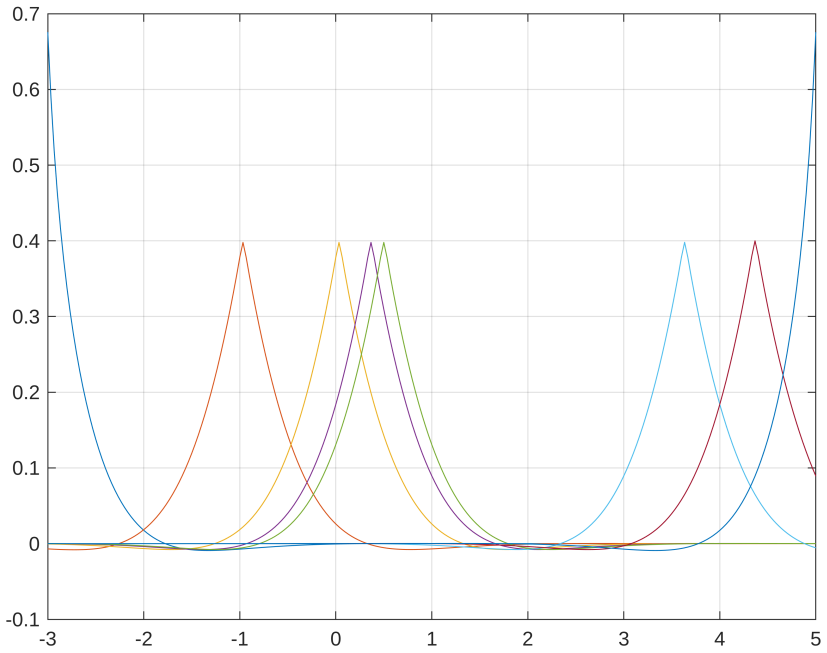
Symmetric square root of covariance matrix

Note that in this case $Q = Q^T = V \cdot \sqrt{D} \cdot V^T$, so this is a "true" square root as $K = Q^2$, no transpose involved.

```
figure()
Q=sqrtm(CovMatrix+1e-13*eye(LL));
norm(Q*Q'-CovMatrix)
```

```
ans = 2.7156e-13
```

```
plot(Xtest,Q(:,[1 62 92 102 106 200 222 241])), grid on
```



When finite window effects have vanished, this would be a "bilateral" convolution kernel that would end up in discrete time as $y(k) = \sum_{s=-\infty}^{+\infty} h(k-s)\xi(s)$, and in continuous time as $y(t) = \int_{-\infty}^{+\infty} h(t-s)\xi(s)\,ds$.

```
function [mu,Var]=predictGP(x1,Data)
arguments
    x1
    Data
end
priormean=@(x) 0.3*x.^2+0.2*x-.2;
lambda=1.5e-2^2; %measurement noise variance
K=@Data.K;
N=length(Data.X);
mu=priormean(x1)';
Var=K(x1,x1); %prior covariance among points in x1
if(N>0) %don't do this if no data available
    K1X=K(x1,Data.X);
    Gain=K1X/(K(Data.X,Data.X)+lambda*eye(N));
    mu=mu+Gain*(Data.Y-priormean(Data.X))';
    Var=Var-Gain*K1X';
    Var=0.5*(Var+Var');
end
end

function km=K(x1,x2)
```

```
M=0.6; sg=0.9;%hyperparameters stddev x and y
%kernel=@(x1,x2) M^2*exp(-norm(x2-x1)^2/2/sg^2); %stationary, depends only
on DIFFERENCE
%kernel=@(x1,x2) M^2*exp(-norm(x2-x1)/sg); %1sr-order exponential
kernel=@(x1,x2) pi*sin(pi/4 + (2^(1/2)*abs(x2-x1))/sg)*exp(-(2^(1/2)*abs(x2-
x1))/sg); %butterworth ord2
N1=length(x1); N2=length(x2); %1D case
km=zeros(N1,N2);
for i=1:N1
    for j=1:N2
        km(i,j)=kernel(x1(:,i),x2(:,j));
    end
end
end
```

```
Varacum=zeros(LL,1);
figure(100)
clf
figure(101)
clf
stddev=norm(Q(1,:));%if stationary
Amplitudes=randn(LL,1);%to build↙
realization by components
shuffle=randperm(LL); %for↙
bilateral simulation
%shuffle=LL:(-1):1;%ANTICAUSAL
%shuffle=1:LL;%not shuffled, for↙
causal or PCA (K-L).
vertflag=true;
for k=1:LL
    i=shuffle(k);
    figure(100)
    Varacum=Varacum+Q(:,i).^2;
    if(k>1)
        plot(Xtest,Q(:,shuffle(1:↙
(k-1))),LineWidth=1)
    end
    hold on
```

```
    plot(Xtest,Q(:,i),LineWidth=3.↙
5), grid on
    if(k>1)
        plot(Xtest,sqrt↙
(Varacum),':k',LineWIdth=2)
        plot(Xtest,-sqrt↙
(Varacum),':k',LineWIdth=2)
    end
    if vertflag
        xline(Xtest(i),'g',↙
LineWidth=2)
    end
    hold off
    title("Component functions↙
(features), scaled by standard↙
dev")
    ylim([-stddev stddev]*1.8)
    fontsize(16,"points") %This↙
works from version 2023a or↙
posterior
    figure(101)
    plot(Xtest,Q(:,i)/max(Q(:,↙
i))), grid on
```

```
    text(-1.9,.25,["i=" num2str(i)↙
num2str(sqrt(eevv(i)))])
    if vertflag
        xline(Xtest(i),'g',↙
LineWidth=2)
    end
    ylim([-1 1])
    title("Component functions↙
(features), scaled to unit↙
amplitude")
    fontsize(16,"points") %This↙
works from version 2023a or↙
posterior
    figure(102)
    for j=1:k %superimpose↙
previous approximations with less↙
components
        RealizTst=Q(:,shuffle(1:↙
j))*Amplitudes(shuffle(1:j));
        if j<k
            plot(Xtest,RealizTst,↙
LineWidth=1,Color=[.9 .95 .7]*((k-↙
j*0.3)/k)^2)
```

```
        else
            plot(Xtest,Q(:,i)↙
*Amplitudes(i),LineWidth=3,Color=↙
[.8 .2 .4])
            plot(Xtest,RealizTst,↙
LineWidth=5+0.04*sqrt(i),Color=[.1↙
.2 .4])
        end
        grid on
        hold on
    end
    ylim([-stddev stddev]*2.65)
     if vertflag
        xline(Xtest(i),'g',↙
LineWidth=2)
    end
    title("Building a realization↙
component by component")
    hold off
    ylabel("Increment with respect↙
to mean")
    fontsize(16,"points") %This↙
works from version 2023a or↙
```

```
posterior
    pause
end
```