```
% Load All The Relavant Data
% Please Change Paths Accordingly
% Senstivity with respect to observations
clc % clear console
clear all % clear all variables from the workspace
% Note windows kind of paths
% loads a matrix that contains prior and lat lon domain of inversion
dataPath='D:\vineet_computer\d_drive\senstivity_paper\section_3.2\';
% Addpath for code files
addpath(genpath(dataPath))
% Load forward  operator, observations and parameters for Q and R
%load([dataPath,'SnspaperData_test_2015_2016_69_70.mat'])
load([dataPath,'data_section_3.2.mat'])
```

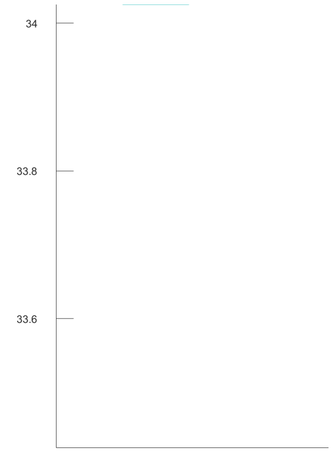
Coordinates of Sites that Measure Methane and other details about observations

```
towerNames={'ONT', 'FUL', 'CMP', 'GRA','USC', 'IRV','CIT','BND'};
timePeriods=2;
% Observation time is stored in amap variable
obsTime=[amap_ONT(:,1) 1*ones(size(amap_ONT,1),1);...% 1 represents ONT
    amap_FUL(:,1) 2*ones(size(amap_FUL,1),1);...% 2 represents FUL
    amap_CMP(:,1) 3*ones(size(amap_CMP,1),1);...
    amap_GRA(:,1) 4*ones(size(amap_GRA,1),1);...
    amap_USC(:,1) 5*ones(size(amap_USC,1),1);...
    amap_UCI(:,1) 6*ones(size(amap_UCI,1),1);...
    amap_PSA(:,1) 7*ones(size(amap_PSA,1),1);...
    amap_BND(:,1) 8*ones(size(amap_BND,1),1)];
% Number of observations available from each tower
towerSize=[size(amap_ONT,1) size(amap_FUL,1) size(amap_CMP,1) ...
    size(amap_GRA,1) size(amap_USC,1) size(amap_UCI,1) size(amap_PSA,1) ...
    size(amap_BND,1)];
% tower coordinates that measures Methane CH4
towerCoord = [34.064167 -117.583611 % Ontario
     33.880417 -117.884122 % Fullerton
     33.873792 -118.276806 % Compton
     34.283889 -118.4725 % Granada Hills
     34.021447 -118.288844 % University of Souther California
     33.644422 -117.844181 % University of California Irvine
     34.1366 -118.12641 % Pasadena
     34.087686 -117.310167]; % San Bernardino
% Time When Observations Were Taken
obsTimePre=[linspace(1,size(H,1),size(H,1))' ...
    obsTime datevec(obsTime(:,1))];
% This would be updated after inversion
obsTimePost=obsTimePre;
obsTowers=num2cell(obsTime(:,2));
% This is just list tower name with each observation time
obsTowers(obsTime(:,2)==1)={'ONT'}; % Ontario
obsTowers(obsTime(:,2)==2)={'FUL'}; % Fullerton
obsTowers(obsTime(:,2)==3)={'CMP'}; % Compton
obsTowers(obsTime(:,2)==4)={'GRA'}; % Granada Hills
```

```
obsTowers(obsTime(:,2)==5)={'USC'}; % University of Souther California
obsTowers(obsTime(:,2)==6)={'UCI'}; % University of California Irvine
obsTowers(obsTime(:,2)==7)={'PSA'}; % Pasadena
obsTowers(obsTime(:,2)==8)={'BND'}; % San Bernardino
```

Plot Spatial Domain or the region of The Study

```
% DOMAIN OF THE STUDY VARIABLES [PLOTTING: NOTHING RELATED TO EQUATIONS]
fluxD=size(H,2)/2;% total no of flux grid cells. Two 4 day time periods
% Create grid of latitude and longitude
% Unique latitudes
uniqueLat=unique(latlon(:,2));
% Unique Longitudes
uniqueLon=unique(latlon(:,1))';
% Grid of Latitude and Longitudes
gridlon1=repmat(uniqueLon,length(uniqueLat),1);
gridlat1=repmat(uniqueLat,1, length(uniqueLon));
% Now we get indices where data would be plotted
% This is the mask
index=zeros(fluxD,2);
for i = 1:fluxD
    [~,col]=min(abs(latlon(i,1)-gridlon1(1,:)));
    [~,row]=min(abs(latlon(i,2)-gridlat1(:,1)));
    index(i,1) = row;
    index(i,2) = col;
end
% This is our plotting grid
mapgrid=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
for i = 1: fluxD
    mapgrid(index(i,1),index(i,2))=1;
end
titles ='Domain of Study';
h=pcolor(gridlon1,gridlat1,mapgrid);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'fontsize',14)
ylabel('Latitude')
xlabel('Longitude')
title(titles,'FontSize', 14,'Fontname','Arial')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','red' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 12,'Fontname','Arial','Color','blue')
hold off
```




```
% Geostat Estimation Equation for Fluxes
% Reference:
% Michalak, Anna M., Lori Bruhwiler, and Pieter P. Tans.
% A geostatistical approach to surface flux
% estimation of atmospheric trace gases. Journal
% of Geophysical Research: Atmospheres 109.D14 (2004).
```

$$\widehat{\mathbf{s}} = \mathbf{X}\widehat{\beta} + \mathbf{QH}^T\Psi^{-1}\left(\mathbf{z} - \mathbf{HX}\widehat{\beta}\right)$$

(Equation 12 in paper)

```
% Definition of Symbols
```

$\hat{\mathbf{s}}$ = fluxes to be estimated (units : micromoles $m^{-2}sec^{-1}$)

$\mathbf{H}$ = forward operator or a jacobian $\left(\text{units} : \frac{\text{ppm}}{\text{micromoles } m^{-2}sec^{-1}}\right)$

$\mathbf{Q}$ = prior error covariance matrix (units : micromoles $m^{-2}sec^{-1})^2$

$\mathbf{X}$ = covariates related to fluxes

$\hat{\beta}$ = weights on covariates *i. e*, $\mathbf{X}$

$\mathbf{z}$ = observations (units : ppm)

$\mathbf{R}$ = observational error covariance or model data mismatach (units : ppm^2)

```
% Dimensions of the Each Quantity/Symbols in the
% Equation
```

$\hat{\mathbf{s}}$ is$(m, 1)$, $\mathbf{H}$ is (n, m), $\mathbf{Q}$ is (k, k), $\mathbf{R}$ is (n, n),
$\mathbf{X}$ is (m, p), $\mathbf{z}$ is $(n, 1)$ and β is $(p, 1)$

```
% We further define:
```

$\mathbf{A} = \mathbf{HX}$, $\Omega = \mathbf{A}^{\mathbf{T}}\Psi^{-1}\mathbf{A}$ and $\Psi^{-1} = \mathbf{HQH}^T + \mathbf{R}$

```
% Replacing Beta in Equation 1 by Equation 2
```

$\hat{\beta} = \Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{z}$

(Equation 13 in Paper)

```
% We get
```

$$\frac{\partial \hat{\mathbf{s}}_G}{\partial \mathbf{z}} = \mathbf{X}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{z} + \mathbf{QH}^{\boldsymbol{T}}\Psi^{-1}(z - \mathbf{A}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{z})$$

(Equation 14)

$$\epsilon = \mathbf{QH}^{\boldsymbol{T}}\Psi^{-1}(z - \mathbf{A}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{z})$$

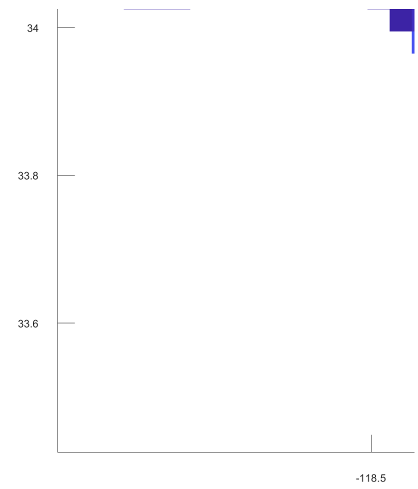
Compute Fluxes From Geostat Method

```
% COMPUTE FLUXES
% All the inputs are in the iput data file
% z are observations
% x is covariance
% R model data mismatch
% Q is prior error covariance
% H is Jacobian Matrix
% By using Eq. 13 & 14  we can compute fluxes as follow:
A=H*X;
psi=H*Q*H'+R;
ipsi=psi\speye(length(psi)); % This expression is
% equivalent to : inverse(psi)
```

```
omega=A'*ipsi*A;
iomega=omega\speye(length(omega)); % This expression is defined in Equation 15 in paper
% equivalent to : inverse(omega)
betaHat = iomega*A'*ipsi*z; % See Eq. 13 in paper
epsilon=Q*H'*ipsi*(z-H*X*betaHat);
shat = X*betaHat+epsilon;% See Eq. 12 in paper
```

Plot Estimated Fluxes

```
% Plot Fluxes [PLOTTING: NOTHING RELATED TO EQUATIONS]
% This is our plotting grid
% For demonstration we plot absolute value of shat as some values of shat
% is negative whereas the CH4 fluxes cannot go negative
mapgrid=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
for i = 1: fluxD
    mapgrid(index(i,1),index(i,2))=abs(shat(i+1826));
end
titles ='Methane Fluxes';
h=pcolor(gridlon1,gridlat1,mapgrid);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'fontsize',14)
caxis([min(abs(shat(1826:end))) max(abs(shat(1826:end)))])
colormap("default")
m=colorbar;
ylabel(m, 'Micromoles m^{-2} sec^{-1}','FontSize', 12,'Fontname','Arial')
set(m,'fontsize',12);
ylabel('Latitude')
xlabel('Longitude')
title(titles,'FontSize', 14,'Fontname','Arial')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment','top',...
    'FontSize', 12,'Fontname','Arial','Color','y')
hold off
```



Compute Senstivity of Estimated Fluxes To Observations $\frac{\partial\,\hat{\mathbf{s}}_G}{\partial\,\mathbf{z}}$

$$\frac{\partial\,\hat{\mathbf{s}}_G}{\partial\,\mathbf{z}} = \mathbf{X}\Omega^{-1}\mathbf{A}^T\Psi^{-1} + \mathbf{Q}\mathbf{H}^T\Psi^{-1} - \mathbf{Q}\mathbf{H}^T\Psi^{-1}\mathbf{A}\Omega^{-1}\mathbf{A}^T\Psi^{-1} = \Lambda$$

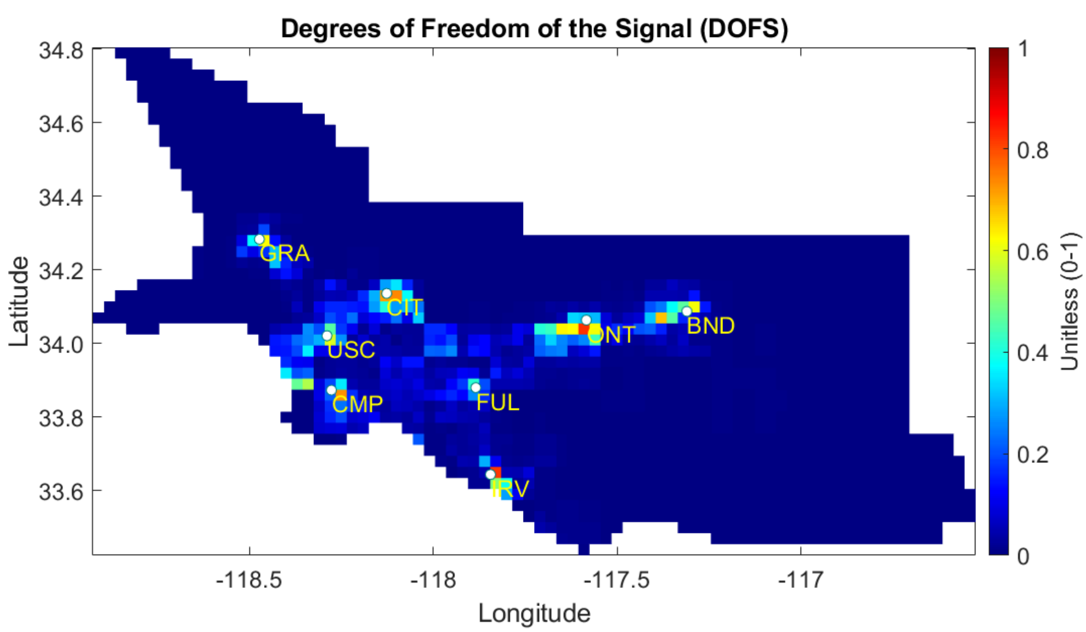
(Equation 17 in paper)

```
% UNITS: (µ Moles m2 sec-1)/ppm
delsG_delZ=(X*iomega*A'*ipsi+Q*H'*ipsi-Q*H'*ipsi*A*iomega*A'*ipsi);
```

Compute and Plot Model Resolution Matrix

```
% Compute
modelRes=(X*iomega*A'*ipsi+Q*H'*ipsi-Q*H'*ipsi*A*iomega*A'*ipsi)*H;
DOFS=(diag(modelRes(1:fluxD,1:fluxD))+diag(modelRes(fluxD+1:fluxD*2,fluxD+1:fluxD*2)))/2;
% PLot
mapgrid=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
```

```
for i = 1: fluxD
    mapgrid(index(i,1),index(i,2))=DOFS(i);
end
titles ='Degrees of Freedom of the Signal (DOFS)';
figure('Renderer', 'painters', 'Position',[16 16 1000 500])
t = tiledlayout(1,1,'TileSpacing','Compact','Padding','Compact');
nexttile
h=pcolor(gridlon1,gridlat1,mapgrid);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'fontsize',14)
caxis([0 1])
colormap("jet")
m=colorbar;
ylabel(m, 'Unitless (0-1)','FontSize', 14,'Fontname','Arial')
ytickformat('%,.1f')
set(m,'fontsize',14);
ylabel('Latitude')
xlabel('Longitude')
title(titles,'FontSize', 14,'Fontname','Arial')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment','top',...
    'FontSize', 14,'Fontname','Arial','Color','y')
hold off
```



Compute $\dfrac{\partial \hat{\mathbf{s}}_G}{\partial \mathbf{X}}$

$$\frac{\partial \widehat{\mathbf{s}}_G}{\partial \mathbf{X}} = \mathbf{K}_z \otimes \left(\mathbf{I} + (\mathbf{M}\mathbf{A}^T - \mathbf{X}\mathbf{\Omega}^{-1}\mathbf{A}^T - \mathbf{Q}\mathbf{H}^T)\mathbf{\Psi}^{-1}\mathbf{H}\right) + (\mathbf{X}\mathbf{\Omega}^{-1} - \mathbf{M}) \otimes \left(\mathbf{F}_z - \mathbf{K}\mathbf{A}^T\mathbf{\Psi}^{-1}\mathbf{H}\right)$$

where

$\mathbf{K}_z = \mathbf{z}^T\mathbf{\Psi}^{-1}\mathbf{A}\mathbf{\Omega}^{-1}$

$\mathbf{M} = \mathbf{Q}\mathbf{H}^T\mathbf{\Psi}^{-1}\ \mathbf{A}\mathbf{\Omega}^{-1}$

$\mathbf{F}_z = \mathbf{z}^T\mathbf{\Psi}^{-1}\mathbf{H}$

Equation(19) in paper

Note we do not $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \mathbf{X}_{\mathrm{ij}}}$ version of the equation as for this smaill problem $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \mathbf{X}}$ can be directly obtained by using Kronecker Form

```
Kz=z'*ipsi*A*iomega;
M=Q*H'*ipsi*A*iomega;
Fz=z'*ipsi*H;
part1=eye(fluxD*timePeriods)+(M*A'-X*iomega*A'-Q*H')*ipsi*H;
part2=X*iomega-M;
part3=Fz-Kz*A'*ipsi*H;
delsG_delX=kron(Kz,part1)+kron(part2,part3);
delsG_delX=full(delsG_delX);
```

Compute $\frac{\partial\, \widehat{\mathbf{s}}_G}{\partial \gamma_i}$ or senstivity with respect to Q parameters.

$$\frac{\partial\, \widehat{\mathbf{s}}_G}{\partial \gamma_i} = \left(-\mathbf{X}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{H} + \mathbf{I}_k - \mathbf{Q}\mathbf{H}^T\Psi^{-1}\mathbf{H} + \mathbf{Q}\mathbf{H}^T\Psi^{-1}\mathbf{A}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{H}\right)\frac{\partial \mathbf{Q}}{\partial \gamma_i}\mathbf{H}^T\Psi^{-1}(\mathbf{z} - \mathbf{A}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{z})$$

Equation 33 in the paper

```
% Compute delsG_delQ Q Units:
% micromoles m^2 sec^-1/(micromoles m^2 sec^-1)^2
% parameters number of parameters for Q
delsG_delGamma=NaN*ones(size(shat,1),size(parameters,1)-length(towerSize));
for i = 1:size(parameters,1)-length(towerSize)
    Q_Qi=eye(length(Q));
    delsG_delGamma(:,i)=(-X*iomega*A'*ipsi*H+eye(size(H,2))-Q*H'*ipsi*H+...
        Q*H'*ipsi*A*iomega*A'*ipsi*H)*Q_Qi*H'*ipsi*(z-A*iomega*A'*ipsi*z);
end
% For an arbitrary full prior covariance matrix a entry by entry
% senstivity can be given as:
```

```
%Note derivative of scalar * identity matrix is just identity matrix
% as given below. This is the form of Q used in this live script and paper
```

$$\mathbf{Q} = \gamma \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

whre γ is a scaling factor optimized through restricted maximum likelihood (REML).

Units of α are $(\text{micromoles } m^{-2}\text{sec}^{-1})^2$

Compute $\frac{\partial\, \widehat{\mathbf{s}}_G}{\partial \alpha_i}$ or senstivity with respect to R parameters.

$$\frac{\partial\, \widehat{\mathbf{s}}_G}{\partial \alpha_i} = \left(-\mathbf{X}\Omega^{-1}\mathbf{A}^T - \mathbf{B} + \mathbf{C}\mathbf{A}\Omega^{-1}\mathbf{A}^T\right)\Psi^{-1}\frac{\partial \mathbf{R}}{\partial \alpha_i}\Psi^{-1}(\mathbf{z} - \mathbf{A}\Omega^{-1}\mathbf{A}^T\Psi^{-1}\mathbf{z})$$

$$\mathbf{B} = \mathbf{Q}\mathbf{H}^T$$

$$\mathbf{C} = \mathbf{B}\Psi^{-1}$$

Equation (31 in the paper)

```
% In this study R for a case study is specified as:
```

$$\mathbf{R} = \begin{bmatrix} \sigma^2_{\text{Tower } A} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma^2_{\text{Tower } A} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma^2_{\text{Tower } B} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma^2_{\text{Tower } B} & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma^2_{\text{Tower } n} \end{bmatrix}$$

```
% Given the structure of delsG_delGamma in Eq. 31 Senstivity
% with respect to particular parameter in R (i.e. delR/delRi) or R_Ri
% like variance for a particular tower specified along a
% diagonal can be specified as:
```

$$\frac{\partial \mathbf{R}}{\partial \alpha_i} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

```
% CODE to compute del shat/del Ri Units: micromoles
% m^2 sec^-1/(ppm)^2
cumtowersize=cumsum(towerSize);
% cumulative sum of total tower observations
```

```
delsG_delalpha=NaN*ones(size(shat,1),length(cumtowersize));
B=Q*H';
C=B*ipsi;
for i = 1: length(towerSize)
    if i == 1 % this step is necessary to get appropriate
        % indices to create derivative matrices
        beginMeas=1;
        endMeas=cumtowersize(i);
    elseif i>1
        beginMeas=cumtowersize(i-1)+1;
        endMeas=cumtowersize(i);
    end
    R_Ri=zeros(size(R,1),1);
    R_Ri(beginMeas:endMeas)=1;
    R_Ri=diag(R_Ri);
    delsG_delalpha(:,i)=(-X*iomega*A'-B+C*A*iomega*A')*...
        ipsi*R_Ri*ipsi*...
        (z-A*iomega*A'*ipsi*z);
end
```

Compute $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \beta}$

$$\frac{\partial \widehat{\mathbf{s}}_G}{\partial \beta} = \mathbf{X} - \mathbf{CA}$$

Equation 20 in the paper

```
delsG_delB=X-C*A;
```

Return Importances Seperately

```
weights_delsdelz = return_importance(delsG_delZ,shat,'sorted');
weights_delsdelR = return_importance(delsG_delalpha,shat,'sorted');
weights_delsdelX = return_importance(delsG_delX,shat,'sorted');
```

Rank Towers

```
cumtowersize=cumsum(towerSize);
indices_ranking=[[1 cumtowersize(1:end-1)+1]' cumtowersize(1:end)'];
totalSum=cell(length(towerSize),2);
totalSum(:,1)=towerNames;
for i=1:length(towerSize)
    iR=find(weights_delsdelz(:,1)>=indices_ranking(i,1) & weights_delsdelz(:,1)<=indices_rankin
    totalSum{i,2}=sum(weights_delsdelz(iR,2));
end
Ranking_Towers=sortrows(totalSum, -2)
```

```
Ranking_Towers = 8×2 cell
```

	1	2
1	'GRA'	0.2564
2	'ONT'	0.2319
3	'CMP'	0.1229
4	'IRV'	0.1044
5	'BND'	0.0910
6	'CIT'	0.0698
7	'FUL'	0.0696
8	'USC'	0.0540

Scale and Combine to find which one of delsdelZ, delsdelR, delsdelX

```
% Note we first scale all the derivatives between 0 and 1 and then sum them
% and once again scale them
```

Scaled derivative of $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \mathbf{z}}$ only one column for z

```
derivative=delsG_delZ;
derivative_scaledZ=(derivative-repmat(min(derivative),size(derivative,1),1)) ./ ...
    (repmat(max(derivative),size(derivative,1),1)-repmat(min(derivative),size(derivative,1),1)
derivative_summed=sum(derivative_scaledZ,2);
delsdelZ_scaled=(derivative_summed-repmat(min(derivative_summed),size(derivative_summed,1),1))
    (repmat(max(derivative_summed),size(derivative_summed,1),1)-repmat(min(derivative_summed),s
```

Scaled derivative of $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \alpha_i}$ only one column for R

```
derivative=delsG_delalpha;
derivative_scaledR=(derivative-repmat(min(derivative),size(derivative,1),1)) ./ ...
    (repmat(max(derivative),size(derivative,1),1)-...
    repmat(min(derivative),size(derivative,1),1));
derivative_summed=sum(derivative_scaledR,2);
delsdelR_scaled=(derivative_summed-repmat(min(derivative_summed),...
    size(derivative_summed,1),1)) ./...
    (repmat(max(derivative_summed),size(derivative_summed,1),1)-...
    repmat(min(derivative_summed),size(derivative_summed,1),1));
```

Scaled derivative of $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \mathbf{X}}$ only one column for X

```
%% Scaled derivative of R
derivative=delsG_delX;
derivative_scaledX=(derivative-repmat(min(derivative),size(derivative,1),1)) ./ ...
    (repmat(max(derivative),size(derivative,1),1)-...
    repmat(min(derivative),size(derivative,1),1));
derivative_summed=sum(derivative_scaledX,2);
delsdelX_scaled=(derivative_summed-repmat(min(derivative_summed),...
    size(derivative_summed,1),1)) ./...
    (repmat(max(derivative_summed),size(derivative_summed,1),1)-...
    repmat(min(derivative_summed),size(derivative_summed,1),1));
```

Scaled derivative of $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \beta}$ only one column for Beta

```
derivative=delsG_delB;
derivative_scaledB=(derivative-repmat(min(derivative),size(derivative,1),1)) ./ ...
    (repmat(max(derivative),size(derivative,1),1)-...
    repmat(min(derivative),size(derivative,1),1));
derivative_summed=sum(derivative_scaledB,2);
delsdelB_scaled=(derivative_summed-repmat(min(derivative_summed),...
    size(derivative_summed,1),1)) ./...
    (repmat(max(derivative_summed),size(derivative_summed,1),1)-...
    repmat(min(derivative_summed),size(derivative_summed,1),1));
```

Scaled derivative of $\frac{\partial \widehat{\mathbf{s}}_G}{\partial \gamma_i}$ only one column for Q

```
derivative=delsG_delGamma;
derivative_scaledQ=(derivative-repmat(min(derivative),size(derivative,1),1)) ./ ...
    (repmat(max(derivative),size(derivative,1),1)-...
    repmat(min(derivative),size(derivative,1),1));
derivative_summed=sum(derivative_scaledQ,2);
delsdelQ_scaled=(derivative_summed-repmat(min(derivative_summed),...
    size(derivative_summed,1),1)) ./...
    (repmat(max(derivative_summed),size(derivative_summed,1),1)-...
    repmat(min(derivative_summed),size(derivative_summed,1),1));
```

Create Independent Variables

```
independent_variables=[delsdelZ_scaled delsdelR_scaled delsdelX_scaled ...
    delsdelQ_scaled delsdelB_scaled];
correlation_evaluation=cell(7);
correlation_evaluation(2:7,2:7)=num2cell(corrcoef([shat independent_variables]));
correlation_names={'variables','shat','delz','delR','delX','delQ','delBeta'};
correlation_evaluation(1,1:7)=correlation_names;
correlation_evaluation(:,1)=correlation_names
```

```
correlation_evaluation = 7×7 cell
```

	1	2	3	4	5	6	7
1	'variables'	'shat'	'delz'	'delR'	'delX'	'delQ'	'delBeta'
2	'shat'	1	0.2985	-0.5594	-0.5004	-0.2159	0.2443
3	'delz'	0.2985	1	-0.0770	-0.3766	-0.1075	0.4695
4	'delR'	-0.5594	-0.0770	1	-0.0726	-0.1797	0.0437
5	'delX'	-0.5004	-0.3766	-0.0726	1	0.2833	-0.3585
6	'delQ'	-0.2159	-0.1075	-0.1797	0.2833	1	-0.2532
7	'delBeta'	0.2443	0.4695	0.0437	-0.3585	-0.2532	1

Get overall importance of z, R, X, Beta, Q

```
% Note index 1 is z, 2 is R, 3 is X, 4 is Beta, 5 is Q
weights_overall = return_importance(independent_variables,shat,'unsorted');
disp('Overall Importance')
```

```
Overall Importance
```

```
Overall_Importance={'z' weights_overall(1,2); 'R' weights_overall(2,2); ...
    'X' weights_overall(3,2); 'Q' weights_overall(4,2);
  'Beta' weights_overall(5,2)}
```

```
Overall_Importance = 5×2 cell
```

	1	2
1	'z'	0.0496
2	'R'	0.5370
3	'X'	0.3134
4	'Q'	0.0646
5	'Beta'	0.0353

```
Overall_Importance=sortrows(Overall_Importance,-2);
```

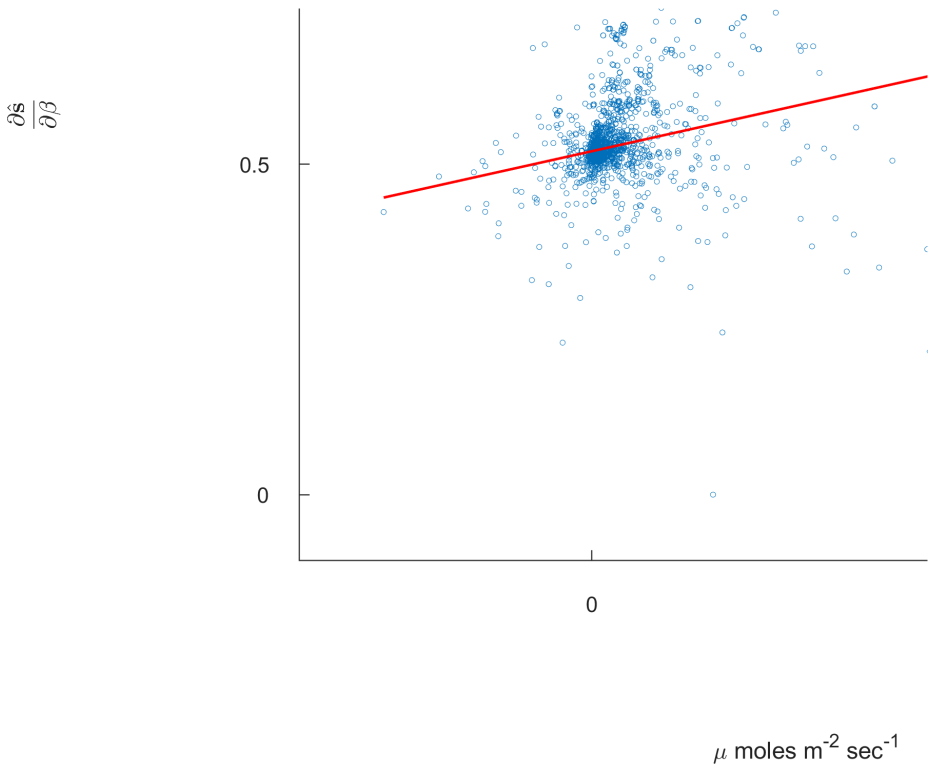
Plot Scatter and Best Fit Line for overall importance

```
close all
% Empty display to create Gap between Figures and Tables of Matrices
disp(' ');
```

```
disp(' ');
```

```
disp(' ');
```

```
fcnCorrMatrixPlot([shat independent_variables], correlation_names(2:end),'Scatterplot matrix of
```



Create Grid Maps for Plotting

```
mapMostImpObs=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapLeastImpObs=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapScaledZ=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapScaledR=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapScaledX=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapScaledQ=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapScaledB=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapgridMost=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapgridHMost=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
mapgridHLeast=ones(size(gridlat1,1),size(gridlon1,2))*NaN;
% because we will plot for onse time period
```

```
H1=H';
for i = 1: fluxD
    mapgridHMost(index(i,1),index(i,2))=H1(i,weights_delsdelz(1,1)) +...
        H1(i+fluxD,weights_delsdelz(1,1));
    mapgridHLeast(index(i,1),index(i,2))=H1(i,weights_delsdelz(end,1))+...
        H1(i+fluxD,weights_delsdelz(end,1));
    mapMostImpObs(index(i,1),index(i,2))=delsG_delZ(i,weights_delsdelz(1,1));
    mapLeastImpObs(index(i,1),index(i,2))=delsG_delZ(i,weights_delsdelz(end,1));
    mapScaledZ(index(i,1),index(i,2))=delsdelZ_scaled(i+1826);
    mapScaledR(index(i,1),index(i,2))=delsdelR_scaled(i+1826);
    mapScaledX(index(i,1),index(i,2))=delsdelX_scaled(i+1826);
    mapScaledQ(index(i,1),index(i,2))=delsdelQ_scaled(i+1826);
    mapScaledB(index(i,1),index(i,2))=delsdelB_scaled(i+1826);
end
```

Plot Most and Least Important Observation

```
% Empty display to create Gap between Figures and Tables of Matrices
disp(' ');
```

```
disp(' ');
```

```
disp(' ');
```

```
close all
figure('Renderer', 'painters', 'Position', [16 16  2200  2000])

subplot(2,2,1)
% z & shat
h=pcolor(gridlon1,gridlat1, mapMostImpObs);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
%text(-117,34.7, ['z = ',num2str(round(z(weights_delsdelz(1,1)),2)) ' ppm'])
set(gca,'Fontsize',16); colormap("default");
m=colorbar;
caxis([min(min(mapMostImpObs)) max(max(mapMostImpObs))])
caxis([0 1])

ylabel(m, '\mu moles m^{-2} sec^{-1}/ppm',...
    'Fontname','Arial','FontSize', 22)
ylabel('Latitude','FontSize', 22); xlabel('Longitude','FontSize', 22)
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
```

```
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
%legend('Enhancement',[num2str(round(z(weights_delsdelz(1,1)),2)) ' ppm']) ;
set(gca,'fontsize',18,'TickDir','in'); colormap("default");
hn=gca;
hn.LineWidth=1.3;
hold off

subplot(2,2,2)
% z & shat
h=pcolor(gridlon1,gridlat1, mapgridHMost);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
m=colorbar;
caxis([min(min(mapgridHMost)) max(max(mapgridHMost))])
ylabel(m, 'ppm/\mu moles m^{-2} sec^{-1}',...
    'Fontname','Arial','FontSize', 18)
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
%legend('z',[num2str(round(z(weights_delsdelz(1,1)),2)), 'ppm']) ;
set(gca,'Fontsize',18,'TickDir','in'); colormap("default");
hn=gca;
hn.LineWidth=1.3;
hold off

subplot(2,2,3)
% z & shat
h=pcolor(gridlon1,gridlat1, mapLeastImpObs);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
m=colorbar;
caxis([min(min(mapLeastImpObs)) max(max(mapLeastImpObs))])
%caxis([min(min(mapMostImpObs)) max(max(mapMostImpObs))])
%caxis([0 1])
ylabel(m, '\mu moles m^{-2} sec^{-1}/ppm',...
    'Fontname','Arial','FontSize', 18)
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
%legend('Enhancement (z; ppm)',num2str(round(z(weights_delsdelz(end,1)),2))) ;
set(gca,'fontsize',18,'TickDir','in'); colormap("default");
```

```
hn=gca;
hn.LineWidth=1.3;
hold off

subplot(2,2,4)
% z & shat
h=pcolor(gridlon1,gridlat1, mapgridHLeast);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'Fontsize',18);
m=colorbar; colormap("default");
caxis([min(min(mapgridHLeast)) max(max(mapgridHLeast))])
ylabel(m, 'ppm/\mu moles m^{-2} sec^{-1}',...
    'Fontname','Arial','FontSize', 18)
%set(m,'Fontsize',22);
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
%legend('Enhancement (z; ppm)', num2str(round(z(weights_delsdelz(end,1)),2))) ;
set(gca,'Fontsize',18,'TickDir','in');
hn=gca;
hn.LineWidth=1.3;
hold off
```

Plot Scaled Derivatives

```
% Empty display to create Gap between Figures and Tables of Matrices
disp(' ');
```

```
disp(' ');
```

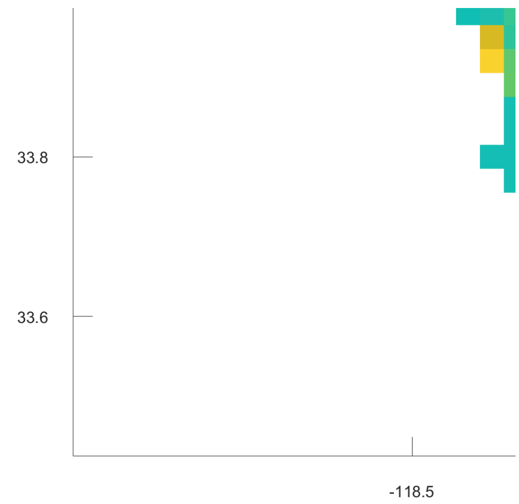
```
disp(' ');
```

```
figure('Renderer', 'painters', 'Position', [16 16  2200  2000])
% f = figure();
% f.WindowState = 'maximized';
```

```
subplot(3,2,1)
% z & shat
h=pcolor(gridlon1,gridlat1, mapScaledZ);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'Fontsize',16); colormap("default");
m=colorbar;
%caxis([min(min(mapScaledZ)) max(max(mapScaledZ))])
caxis([0 1])
ylabel(m, 'Unitless 0-1',...
    'Fontname','Arial','FontSize', 18)
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
title('$$\frac{\partial \hat{\mathbf{s}} }{\partial \mathbf{z}}$$','interpreter','latex','FontS
set(gca,'fontsize',18,'TickDir','in'); colormap("default");
hold off

subplot(3,2,2)
% z & shat
h=pcolor(gridlon1,gridlat1, mapScaledR);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
m=colorbar;
%caxis([min(min(mapScaledR)) max(max(mapScaledR))])
caxis([0 1])
ylabel(m, 'Unitless 0-1',...
    'Fontname','Arial','FontSize', 18)
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
title('$$\frac{\partial \hat{\mathbf{s}} }{\partial \mathbf{R}}$$','interpreter','latex','FontS
set(gca,'Fontsize',18,'TickDir','in'); colormap("default");
hold off

subplot(3,2,3)
% z & shat
h=pcolor(gridlon1,gridlat1, mapScaledX);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
```

```
axis image;   % real x,y scaling
m=colorbar;
%caxis([min(min(mapScaledX)) max(max(mapScaledX))])
caxis([0 1])
ylabel(m, 'Unitless 0-1',...
    'Fontname','Arial','FontSize', 18)
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
title('$$\frac{\partial \hat{\mathbf{s}} }{\partial \mathbf{X}}$$','interpreter','latex','FontS
set(gca,'fontsize',18,'TickDir','in'); colormap("default");
hold off

subplot(3,2,4)
% z & shat
h=pcolor(gridlon1,gridlat1,  mapScaledQ);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'Fontsize',18);
m=colorbar; colormap("default");
%caxis([min(min( mapScaledQ)) max(max( mapScaledQ))])
caxis([0 1])
ylabel(m, 'Unitless 0-1',...
    'Fontname','Arial','FontSize', 18)
%set(m,'Fontsize',22);
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
title('$$\frac{\partial \hat{\mathbf{s}} }{\partial \mathbf{Q}}$$','interpreter','latex','FontS
set(gca,'Fontsize',18,'TickDir','in');
hold off

subplot(3,2,5.5)
% z & shat
h=pcolor(gridlon1,gridlat1,  mapScaledB);
set(h, 'EdgeColor', 'none');
shading flat; % do not interpolate pixels
axis on;      % display axis
axis tight;   % no white borders
axis image;   % real x,y scaling
set(gca,'Fontsize',18);
m=colorbar; colormap("default");
%caxis([min(min( mapScaledQ)) max(max( mapScaledQ))])
caxis([0 1])
ylabel(m, 'Unitless 0-1',...
```

```
    'Fontname','Arial','FontSize', 18)
%set(m,'Fontsize',22);
ylabel('Latitude'); xlabel('Longitude')
hold on
plot(towerCoord(:,2), towerCoord(:,1),'o','MarkerEdgeColor',[0 .5 .5],...
    'MarkerFaceColor','auto' );
text(towerCoord(:,2),towerCoord(:,1),towerNames,'VerticalAlignment',...
    'top','FontSize', 16,'Fontname','Arial','Color','y')
title('$$\frac{\partial \hat{\mathbf{s}} }{\partial \mathbf{\beta}}$$','interpreter','latex','F
set(gca,'Fontsize',18,'TickDir','in');
hold off
```




```
% Multivatiate Taylor Series Normalization Based
% on Variances
```

Consider $\hat{s} = f(Q,R,H,X,z) := f\left(Q\left(\theta_{Q_1},\cdots,\theta_{Q_l}\right), R\left(\theta_{R_1},\cdots,\theta_{R_m}\right), H\left(\theta_{H_1},\cdots,\theta_{H_n}\right), X\left(\theta_{X_1},\cdots,\theta_{X_o}\right), z\left(\theta_{z_1},\cdots,\theta_{z_p}\right)\right)$

i.e. it can be written as

$$f(Q,R,H,X,z) = f\left(\underbrace{\theta_{Q_1},\cdots,\theta_{Q_l}}_{\theta_Q},\underbrace{\theta_{R_1},\cdots,\theta_{R_m}}_{\theta_R},\underbrace{\theta_{H_1},\cdots,\theta_{H_n}}_{\theta_H},\underbrace{\theta_{X_1},\cdots,\theta_{X_o}}_{\theta_X},\underbrace{\theta_{z_1},\cdots,\theta_{z_p}}_{\theta_z}\right)$$

then by Multivariate Taylor's series expansion, $V_{\hat{s}}$ can be expressed as

$$V_{\hat{s}} = \left(\frac{\partial\hat{s}}{\partial\theta_Q},\frac{\partial\hat{s}}{\partial\theta_R},\frac{\partial\hat{s}}{\partial\theta_H},\frac{\partial\hat{s}}{\partial\theta_X},\frac{\partial\hat{s}}{\partial\theta_z}\right)_{\theta=\hat{\theta}}\begin{pmatrix} V_{\hat{\theta}_Q} & Cov(\hat{\theta}_Q,\hat{\theta}_R) & Cov(\hat{\theta}_Q,\hat{\theta}_H) & Cov(\hat{\theta}_Q,\hat{\theta}_X) & Cov(\hat{\theta}_Q,\hat{\theta}_z) \\ Cov(\hat{\theta}_R,\hat{\theta}_Q) & V_{\hat{\theta}_R} & Cov(\hat{\theta}_R,\hat{\theta}_H) & Cov(\hat{\theta}_R,\hat{\theta}_X) & Cov(\hat{\theta}_R,\hat{\theta}_z) \\ Cov(\hat{\theta}_H,\hat{\theta}_Q) & Cov(\hat{\theta}_H,\hat{\theta}_R) & V_{\hat{\theta}_H} & Cov(\hat{\theta}_H,\hat{\theta}_X) & Cov(\hat{\theta}_H,\hat{\theta}_z) \\ Cov(\hat{\theta}_X,\hat{\theta}_Q) & Cov(\hat{\theta}_X,\hat{\theta}_R) & Cov(\hat{\theta}_X,\hat{\theta}_H) & V_{\hat{\theta}_X} & Cov(\hat{\theta}_X,\hat{\theta}_z) \\ Cov(\hat{\theta}_z,\hat{\theta}_Q) & Cov(\hat{\theta}_z,\hat{\theta}_R) & Cov(\hat{\theta}_z,\hat{\theta}_H) & Cov(\hat{\theta}_z,\hat{\theta}_X) & V_{\hat{\theta}_z} \end{pmatrix}\left(\frac{\partial\hat{s}}{\partial\theta_Q},\frac{\partial\hat{s}}{\partial\theta_R},\frac{\partial\hat{s}}{\partial\theta_H},\right.$$

To compare Q and R parameters, we can disregard other parameters and write it as:

$$V_{\hat{s}} = \left(\frac{\partial\hat{s}}{\partial\theta_Q},\frac{\partial\hat{s}}{\partial\theta_R}\right)_{\theta=\hat{\theta}}\begin{pmatrix} V_{\hat{\theta}_Q} & Cov(\hat{\theta}_Q,\hat{\theta}_R) \\ Cov(\hat{\theta}_R,\hat{\theta}_Q) & V_{\hat{\theta}_R} \end{pmatrix}\left(\frac{\partial\hat{s}}{\partial\theta_Q},\frac{\partial\hat{s}}{\partial\theta_R}\right)^T_{\theta=\hat{\theta}} + \text{Error}$$

$$V_{\hat{s}} \approx \left(\frac{\partial\hat{s}}{\partial\theta_Q}V_{\hat{\theta}_Q}\frac{\partial\hat{s}}{\partial\theta_Q}^T + \frac{\partial\hat{s}}{\partial\theta_R}V_{\hat{\theta}_R}\frac{\partial\hat{s}}{\partial\theta_R}^T\right)_{\theta=\hat{\theta}} \qquad \text{when the covariance terms are 0}$$

Then the diagonal of the variance of posterior fluxes can be written as

$$Var(s_i) = \left(\left(\frac{\partial\hat{s}}{\partial\theta_{Q_1}}\right)_i^2 V_{\theta_{Q_1}} + \cdots + \left(\frac{\partial\hat{s}}{\partial\theta_{Q_1}}\right)_i^2 V_{\theta_{Q_l}}\right)_{\theta=\hat{\theta}} + \left(\left(\frac{\partial\hat{s}}{\partial\theta_{R_1}}\right)_i^2 V_{\theta_{R_1}} + \cdots + \left(\frac{\partial\hat{s}}{\partial\theta_{R_m}}\right)_i^2 V_{\theta_{R_m}}\right)_{\theta=\hat{\theta}} \qquad \text{where } ()_i \text{ denotes ith elemen}$$

We can combine these individual contributions in the following way for comparison:

$$\begin{aligned} Var(s_i) &= \left(\left(\frac{\partial\hat{s}}{\partial\theta_{Q_1}}\right)_i^2 V_{\theta_{Q_1}},\cdots,\left(\frac{\partial\hat{s}}{\partial\theta_{Q_1}}\right)_i^2 V_{\theta_{Q_l}},\left(\frac{\partial\hat{s}}{\partial\theta_{R_1}}\right)_i^2 V_{\theta_{R_1}},\cdots,\left(\frac{\partial\hat{s}}{\partial\theta_{R_m}}\right)_i^2 V_{\theta_{R_m}}\right)_{\theta=\hat{\theta}} \qquad \text{where } ()_i \text{ denotes ith element of the vector} \\ &= (D_{i1},D_{i2},\cdots,D_{il+m}) \end{aligned}$$

```
% First formulate Variance in diag
varRQ=diag(inv(fisher));
varRQ=diag([varRQ(1:end-1); varRQ(end)]);
% Keep contributions in a matrix (#rows=#fluxes,#columns=#parameters)
contribs=zeros(length(parameters),1);
vartheta=diag(varRQ);
delsdelRQ=[delsG_delalpha delsG_delGamma];
totalFluxes=size(delsdelRQ,1);

for i=1:totalFluxes
    for j=1:size(parameters,1)
        contribs(i,j)= delsdelRQ(i,j).^2 * vartheta(j);
    end
end

% Obtain relative contribution of the Q and R parameters ...
```

```
% onto posterior uncertainty
G=sum(contribs);
disp(['Relative contribution of flux sensitivities w.r.t R ...' ...
    'and Q parameters on posterior variance'])
```

```
Relative contribution of flux sensitivities w.r.t R ...and Q parameters on posterior variance
```

```
G./sum(G)
```

```
ans = 1×9
    0.9998    0.0000    0.0000    0.0000    0.0000    0.0001    0.0000    0.0001 ⋯
```

```
clear A amap* ans Area Fit F f H_* z_* part* ipsi iomega nfluxes nFluxes ...
    noTowers obs* psi Qderiv Rderiv XQR rtowers row omega ...
dataPath begin* betaHat* col cumtowersize derivative_scaled ...
derivative_summed endMeas i derivative titles mapgrid K m uniqueLat ...
uniqueLon timePeriods towerSize parameters mask h M dates_
```