Question 1

```
In[∘ ]:= Needs["NumericalCalculus`"]
Clear[NDSolveAround]
NDSolveAround[eqns_, params___, opts : OptionsPattern[]] :=
 Module[{nn, NDRules, i, ΔΔ, X, xs, xsrules, Δs, consts, symbols, pairs, rules, efun, F, F0, G,
   means, errors, M, a, b, NDD, FD, outseries, MeanOutSeries, ErrorOutSeries, outrules},
  (* Option settings and checks *)
  nn = OptionValue["AroundReplaceOrder"];
  If[(Method /. OptionValue["NDOptions"]) ≠ EulerSum ∧
    (Method /. OptionValue["NDOptions"]) ≠ Method,
   Message[NDSolveAround::InvalidNDMethod, Method /. OptionValue["NDOptions"]],
   Null, Message[NDSolveAround::InvalidNDMethod, Method /. OptionValue["NDOptions"]]];
  NDRules = OptionValue["NDOptions"] /. (Rule[Method, a_] → Rule[Method, EulerSum]);
  (* First find constants that have error *)
  consts = DeleteDuplicates[Cases[eqns, a_Around, ∞]];
  (* Make symbols and pair them with the consts *)
  symbols = Table[Unique[], {i, 1, Length[consts]}];
  pairs = List @@ GroupBy[{consts, symbols}ᵀ, First];
  rules = MapThread[#1 → #2 &, {consts, symbols}];
  (* Make a function which takes consts as inputs and returns eqns with these consts *)
  efun = Function[Evaluate[symbols], Evaluate[eqns /. rules]];
  (* Next we treat the output of NDSolve as a function,
  and propagate error through it based on its derivatives *)
  F[vals_] :=
   F[vals] = NDSolveValue[efun @@ vals, params, FilterRules[{opts}, Options[NDSolve]]];
  means = #["Value"] & /@ consts;
  errors = #["Uncertainty"] & /@ consts;
  F0 = F[means];
  M = Length[F0];
  (* Make a function to compute finite
   difference expressions for higher mixed partials *)
  xs = Table[Unique[X], {k, 1, Length[consts]}];
  Δs = Table[Unique[ΔΔ], {k, 1, Length[consts]}];
  xsrules = MapThread[Rule, {xs, means}];
  FD[f_, {i_, n_}] := FD[f, i] = Function[Evaluate[xs],
     Evaluate[(ND[f @@ xs, {xs[[i]], n}, xs[[i]], Sequence @@ NDRules])]];
  NDD[f_, l_] := Module[{out},
    out = f;
    For[i = 1, i ≤ Length[l], i++,
     out = FD[out, {i, l[[i]]}]
    ];
    out
   ];
  (* Use these functions to compute the outvalue and outerrors *)
```

```
outseries = AroundReplace[G[Sequence @@ xs],
    Evaluate[Table[xs〚i〛 → Around[xs〚i〛, Δs〚i〛], {i, 1, Length[xs]}]], nn];
  MeanOutSeries = outseries["Value"];
  ErrorOutSeries = outseries["Uncertainty"];
  outrules = MapThread[#1 → #2 &, {Δs, errors}];
  Table[Evaluate[(Around[MeanOutSeries, ErrorOutSeries] /.
          {G[__] :> F0〚m〛[b], G^(s__)[__] :> (NDD[a, {s}] @@ means)} /.
         a[x__] :> F[{x}]〚m〛[b]) /. b → ##] &, {m, 1, M}] /. outrules

 ]

Options[NDSolveAround] = Join[{
     "AroundReplaceOrder" → 1,
     "NDOptions" → {Method → EulerSum}
    }, Options[NDSolve]];
NDSolveAround::InvalidNDMethod =
  "EulerSum is currently the only supported ND method, Method → `1` will be ignored.";
```

a)

There is a type of bimolecular chemical reaction known as the ”Brusselator” which is governed by the following ordinary differential equations:

$$\frac{\partial}{\partial t}X(t) = A + X(t)^2Y(t) - BX(t) - X(t) \tag{1}$$

$$\frac{\partial}{\partial t}Y(t) = BX(t) - X(t)^2Y(t) \tag{2}$$

Experimental data measuring the values of X and Y over time is shown in Table 1. Using these data points and least squares regression, find the values of A and B from equations 1 and 2 which fit the data the best.

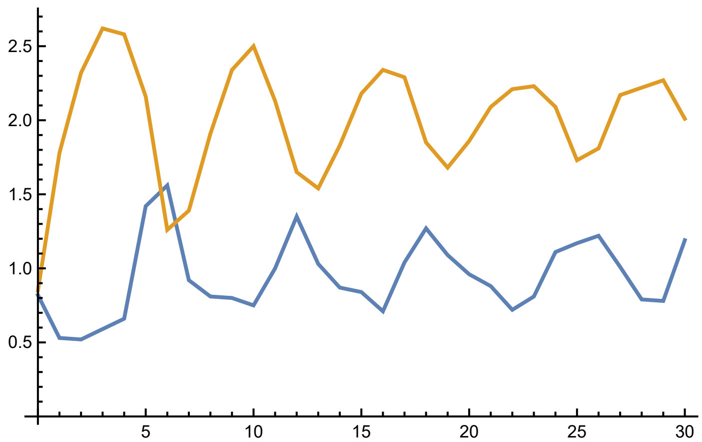
In[ ]:=
```
Partition[ToExpression@StringSplit["0 0.82 0.85
1 0.53 1.78
2 0.52 2.32
3 0.59 2.62
4 0.66 2.58
5 1.42 2.16
6 1.56 1.26
7 0.92 1.39
8 0.81 1.91
9 0.8 2.34
10 0.75 2.5
11 1 2.13
12 1.35 1.65
13 1.03 1.54
14 0.87 1.83
15 0.84 2.18
16 0.71 2.34
17 1.04 2.29
18 1.27 1.85
19 1.09 1.68
20 0.96 1.86
21 0.88 2.09
22 0.72 2.21
23 0.81 2.23
24 1.11 2.09
25 1.17 1.73
26 1.22 1.81
27 1.01 2.17
28 0.79 2.22
29 0.78 2.27
30 1.19 2.01"], 3] // Iconize
```

Out[ ]=
```
{⋯} +
```

In[ ]:=
```
data = {⋯} + ;
```

In[∘]:=
```
ListLinePlot[{data /. {t_, X_, Y_} :→ {t, X}, data /. {t_, X_, Y_} :→ {t, Y}}]
```

Out[∘]=



In[∘]:=
```
ClearAll[SolveSystem, Xfun, Yfun]
SolveSystem[A_?NumericQ, B_?NumericQ] := SolveSystem[A, B] = Module[{},
   NDSolveValue[{
     X'[t] == A + X[t]^2 Y[t] - B X[t] - X[t],
     Y'[t] == B X[t] - X[t]^2 Y[t],
     X[0] == data[[1, 2]],
     Y[0] == data[[1, 3]]
    }, {X, Y}, {t, 0, 31}]
  ]
Xfun[A_?NumericQ, B_?NumericQ, t_?NumericQ] := SolveSystem[A, B][[1]][t]
Yfun[A_?NumericQ, B_?NumericQ, t_?NumericQ] := SolveSystem[A, B][[2]][t]
```

In[∘]:=
```
MultiNonlinearModelFit = ResourceFunction["MultiNonlinearModelFit"];
```

In[∘]:=
```
model = MultiNonlinearModelFit[
  Evaluate[{data /. {t_, X_, Y_} :→ {t, X}, data /. {t_, X_, Y_} :→ {t, Y}}],
  {Xfun[A, B, t], Yfun[A, B, t]}, {A, B}, t,
  Method → {"NMinimize", Method → "SimulatedAnnealing"}]
```

Out[∘]=

```
FittedModel[ Switch[Round[n], 1, Xfun[1.00842, 1.99868, t], 2, Yfun[1.00842, 1.99868, t]] ]
```

In[∘]:=
```
model["ParameterConfidenceIntervalTable"]
```

Out[∘]=

	Estimate	Standard Error	Confidence Interval
A	1.00842	0.003082	{1.00225, 1.01458}
B	1.99868	0.0119422	{1.9748, 2.02257}

In[∘]:=
```
{Aval, Bval} = Around @@@ ({Values@model["BestFitParameters"], model["ParameterErrors"]}ᵀ)
```

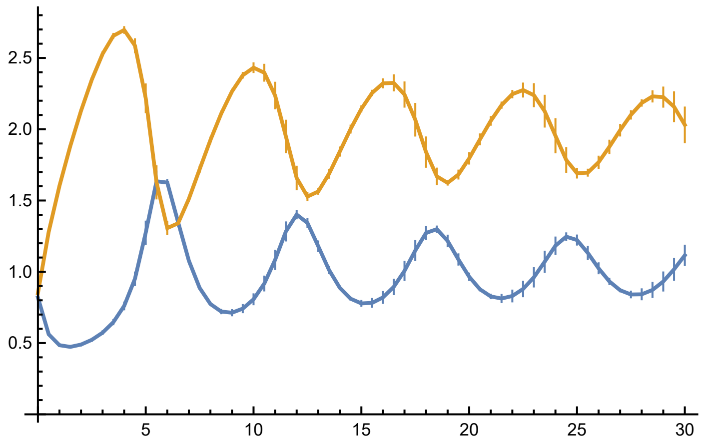
Out[∘]=

{1.0084 ± 0.0031, 1.999 ± 0.012}

In[ ]:=
```
sol = NDSolveAround[{
    X'[t] == Aval + X[t]^2 Y[t] - Bval X[t] - X[t],
    Y'[t] == Bval X[t] - X[t]^2 Y[t],
    X[0] == data[[1, 2]],
    Y[0] == data[[1, 3]]
   }, {X, Y}, {t, 0, 31}, "AroundReplaceOrder" → 1];
```

In[ ]:=
```
ListLinePlot[
 {Table[{t, sol[[1]][t]}, {t, 0, 30, 0.5}], Table[{t, sol[[2]][t]}, {t, 0, 30, 0.5}]}]
```

Out[ ]=



Question 2

Question 2

Assuming that A = 2 and B = 5 and that X[0] = Y[0] = 1 find the average value of X and Y from time t=0 to t=30

In[ ]:=
```
A = 2;
B = 5;
sol = NDSolve[{
    X'[t] == A + X[t]^2 Y[t] - B X[t] - X[t],
    Y'[t] == B X[t] - X[t]^2 Y[t],
    X[0] == 1,
    Y[0] == 1
   }, {X, Y}, {t, 0, 31}];
```

In[ ]:=
```
Xavg = 1/30 NIntegrate[X[t] /. sol[[1]], {t, 0, 30}];
Yavg = 1/30 NIntegrate[Y[t] /. sol[[1]], {t, 0, 30}];
```

In[ ]:=
```
Plot[Evaluate[{X[t], Y[t], Xavg, Yavg} /. sol], {t, 0, 30}, PlotRange → All]
```

Out[ ]=