pyGAM

balancing predictive power and interpretability with generalized additive models

dani servén marín

Who are you?

- twin
- Spain + USA
- <3
  - Full-stack data (ml, r+d, deploying...)
  - Society + environment
  - learning
  - open source
  - d.i.y
- core contributor to pyGAM

github.com/dswah/

What's pyGAM?

New open-source library for estimating Generalized Additive Models.

- Modular
- Pure Python
- Plays nice with PyData tools

github.com/dswah/pygam

Compatible with sklearn

```
# do regression
gam = LinearGAM().fit(X, y)
y_pred = gam.predict(X)


# or do classification
lgam = LogisticGAM().fit(X, y)
lgam.accuracy(X, y)


# build a custom model
custom_gam = GAM(link='log', distribution='poisson').fit(X, y)
```

Why did you make pyGAM?

- No P-spline GAMs in Python
- Contribute to PyData stack

Why did you make pyGAM?

Human learning:

- Statistics
- Code quality
- Open-source

Not enough time...

Regression

Confidence intervals

Prediction intervals

Partial dependence

Model statistics

Classification

Custom GAMs

Sampling from fitted models

Extrapolation

Monotonic / Convex / Concave constraints

Histogram smoothing

Weighted data

Sklearn RandomizedSearchCV

Alternate optimization objectives

Optimizer Callbacks

Expectiles

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Welcome to PyDatatopolis

Need to generate power for our self-sufficient city

- Plan tomorrow's hourly power demand
- too low => blackouts
- too high => waste resources
- Data Driven™

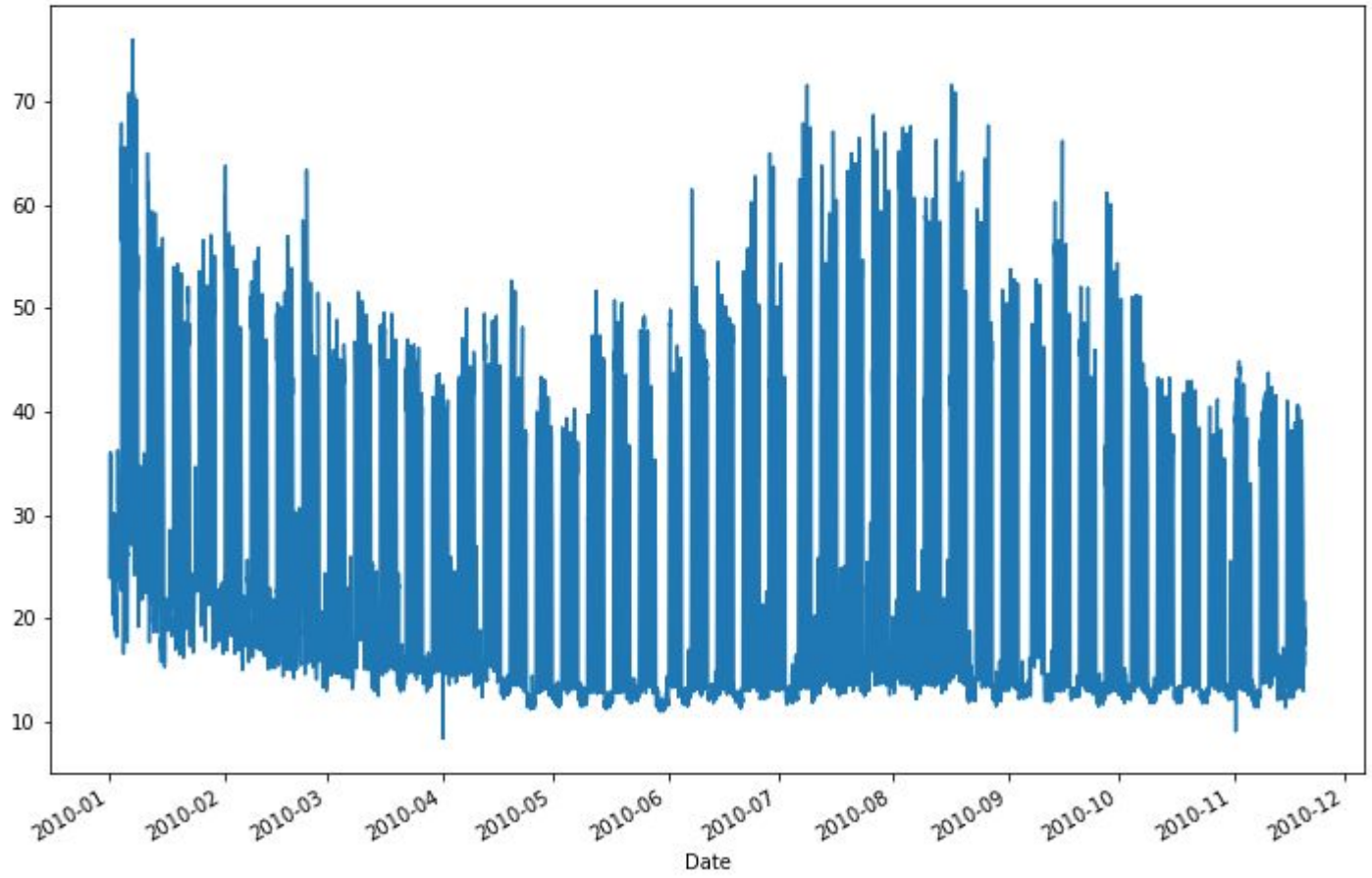
Welcome to PyDatatopolis

```
df.columns
```

```
Index(['OAT', 'Building 6 kW', 'Cloud Cover'], dtype='object')
```

```
df['Building 6 kW'].plot(figsize=(12,8))
```

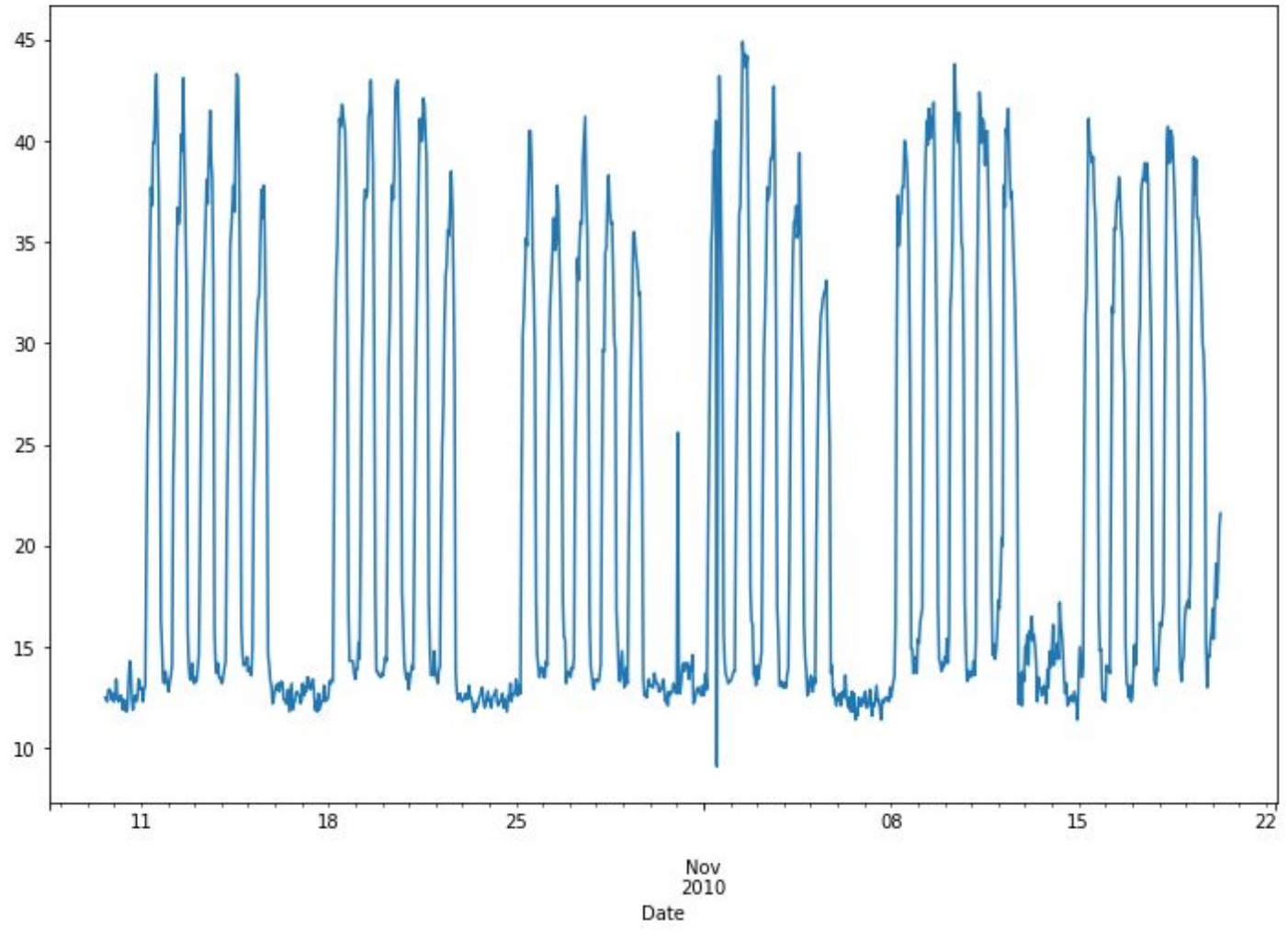
```
<matplotlib.axes. subplots.AxesSubplot at 0x7f8aa72d57b8>
```



Welcome to PyDatatopolis

```
df['Building 6 kW'][-1000:].plot(figsize=(12,8))
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x7feeaac56b00>
```



Welcome to PyDatatopolis

- Build LSTM / ARIMAX / kNN / ... model
- Good fit
- Show your comrades the prediction for tomorrow
- But they are skeptical...

Welcome to PyDatatopolis

- How certain are you?
- It's going to be a hot summer
  - how should we prepare?...
- What happens on sunny days?
- etc?

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You survey your tool box...

- Linear models have too much bias
- Powerful models are black boxes
- ARIMAX just gives you coefficients
- ...

Welcome to PyDatatopolis

You take a break...

read a blog post about GAMs

Welcome to PyDatatopolis

You take a break...

read a blog post about GAMs

so you try it out…

```
pip install pygam
```

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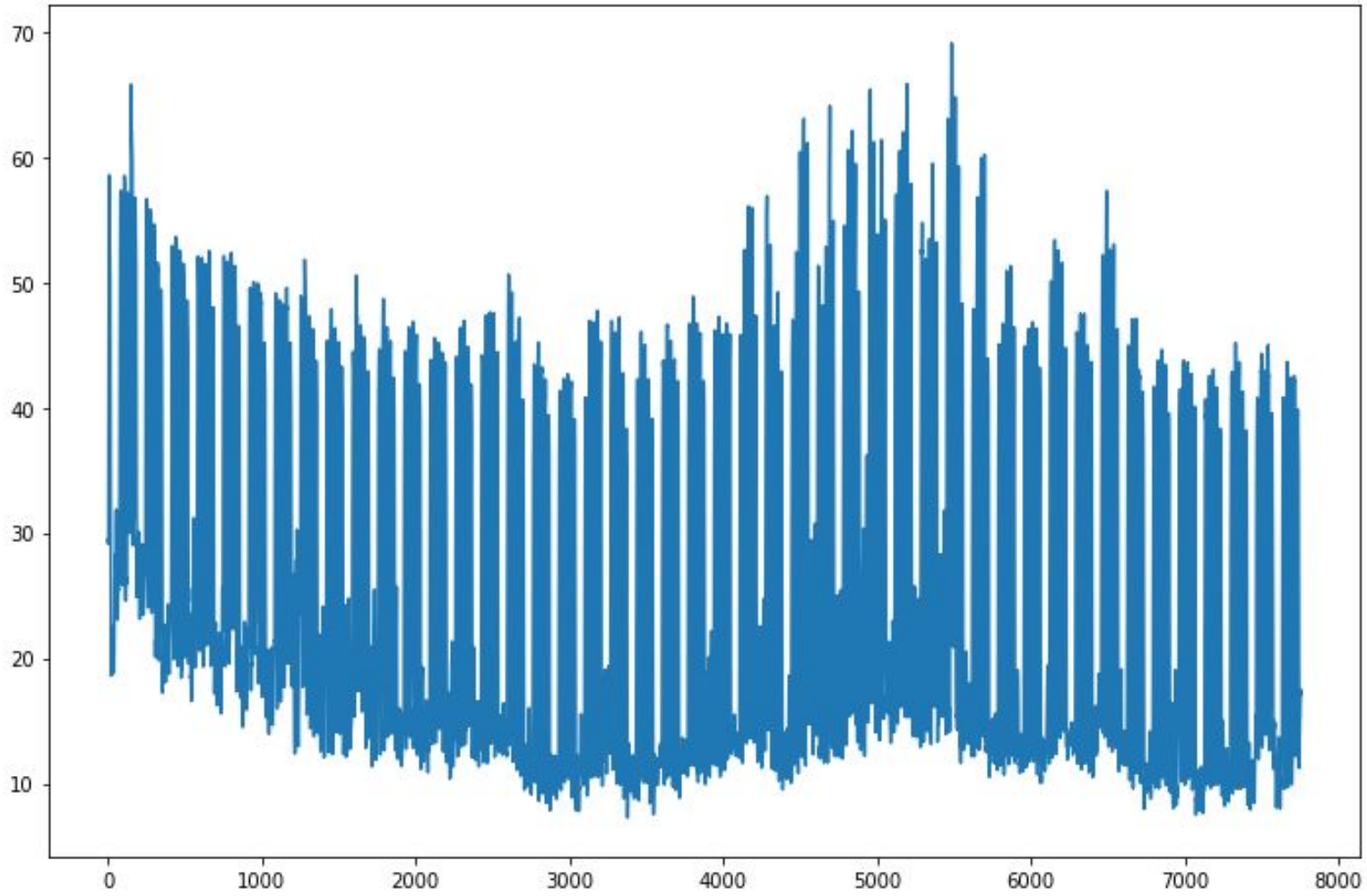
```
X = df[['day_of_week', 'time_of_year', 'OAT', 'Cloud Cover']].values
y = df['Building 6 kW'].values

from pygam import LinearGAM
gam = LinearGAM().fit(X, y)
```

Welcome to PyDatatopolis

```
plt.plot(gam.predict(X))
```

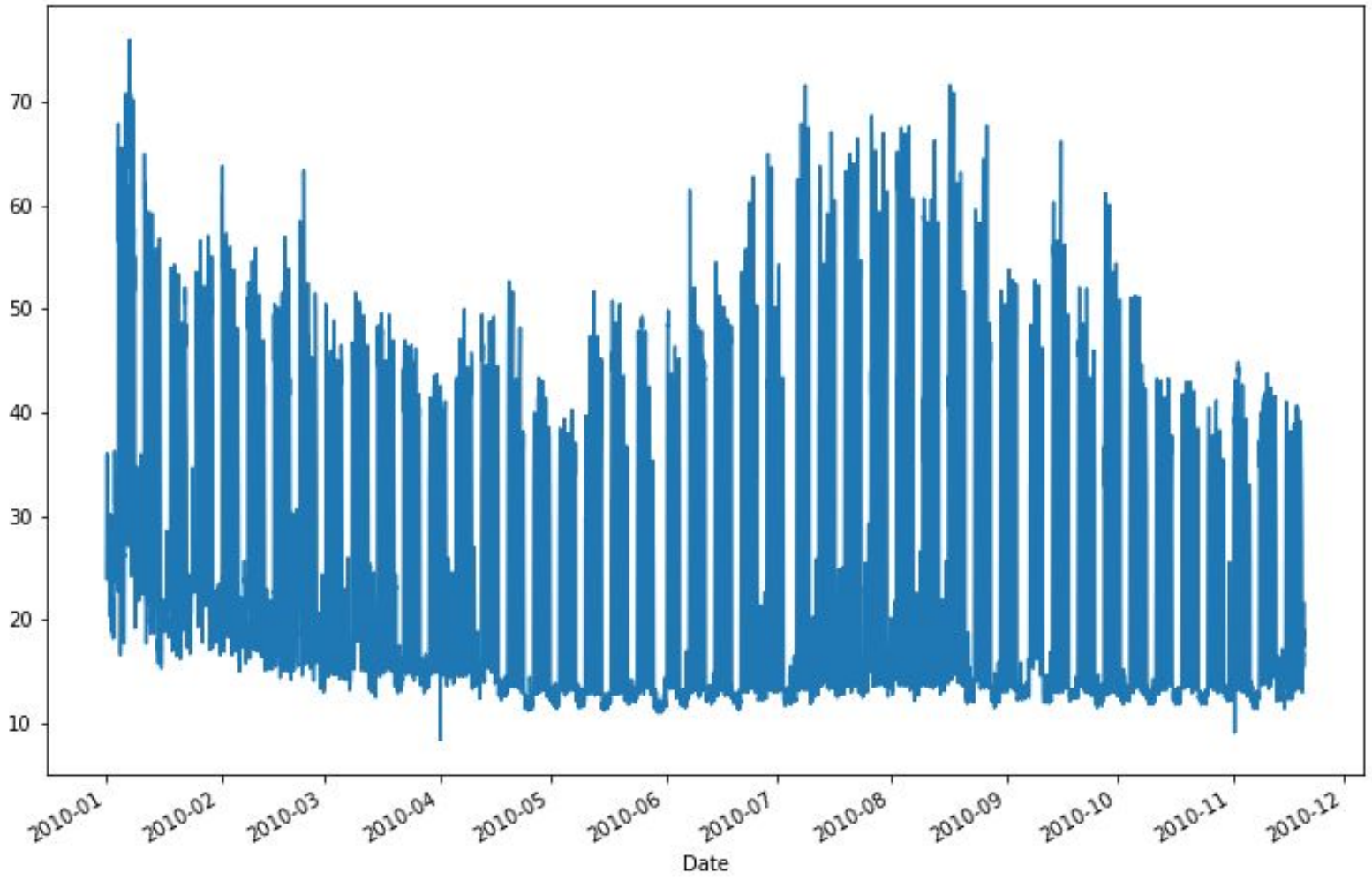
```
[<matplotlib.lines.Line2D at 0x7feea8128ba8>]
```



Welcome to PyDatatopolis

```
df['Building 6 kW'].plot(figsize=(12,8))
```

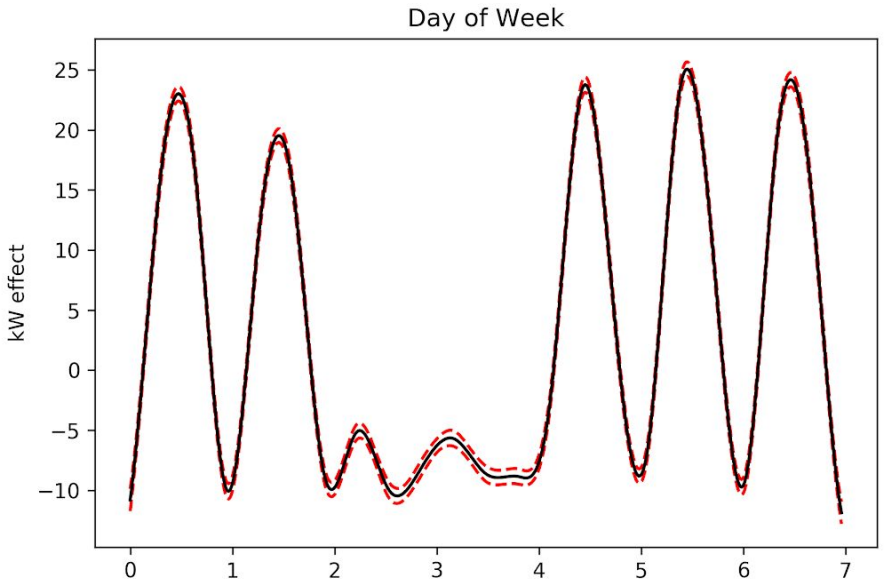
```
<matplotlib.axes. subplots.AxesSubplot at 0x7f8aa72d57b8>
```

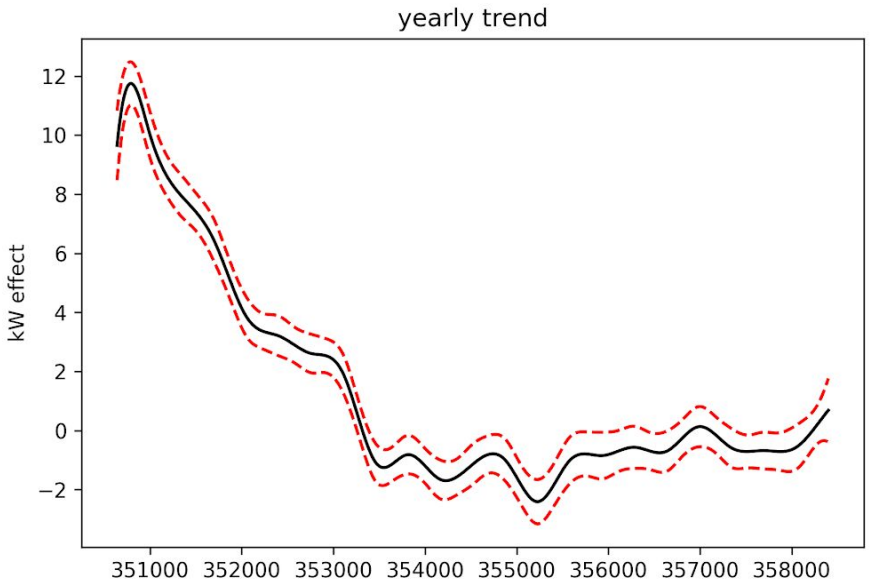


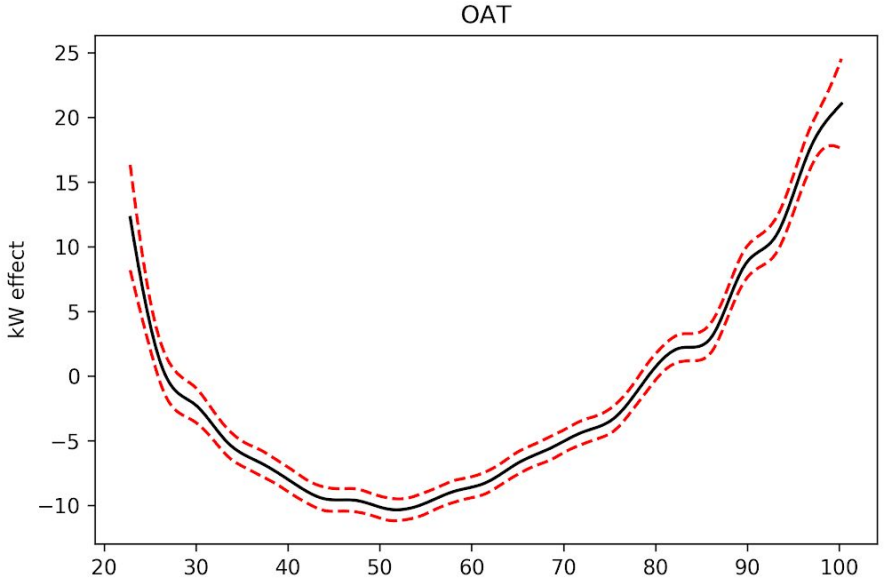
What's pyGAM?

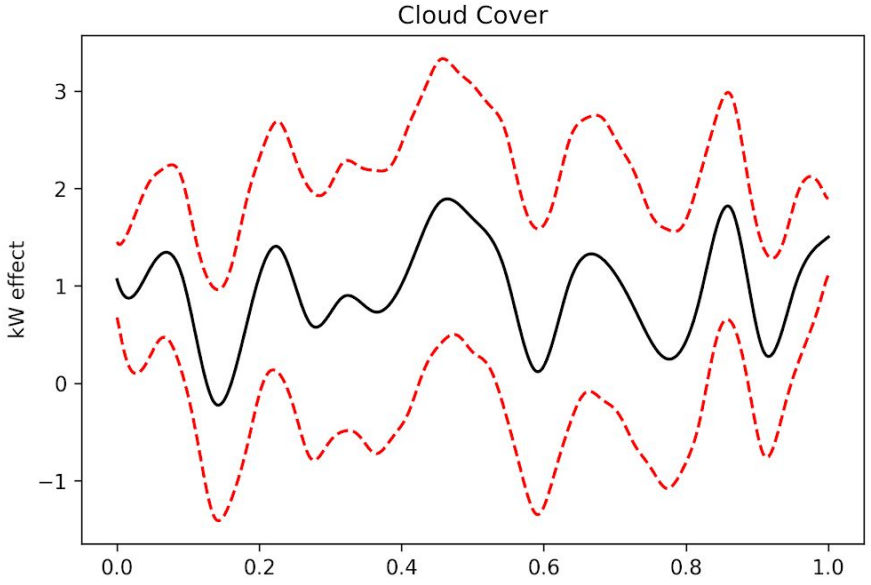
```
pdeps, confi = gam.partial_dependence(width=0.95)
```

Welcome to PyDatatopolis





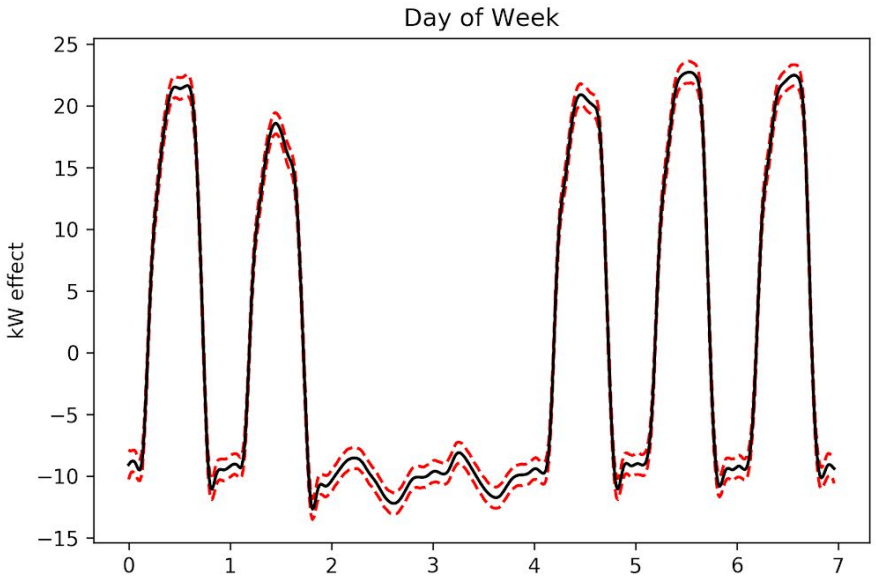


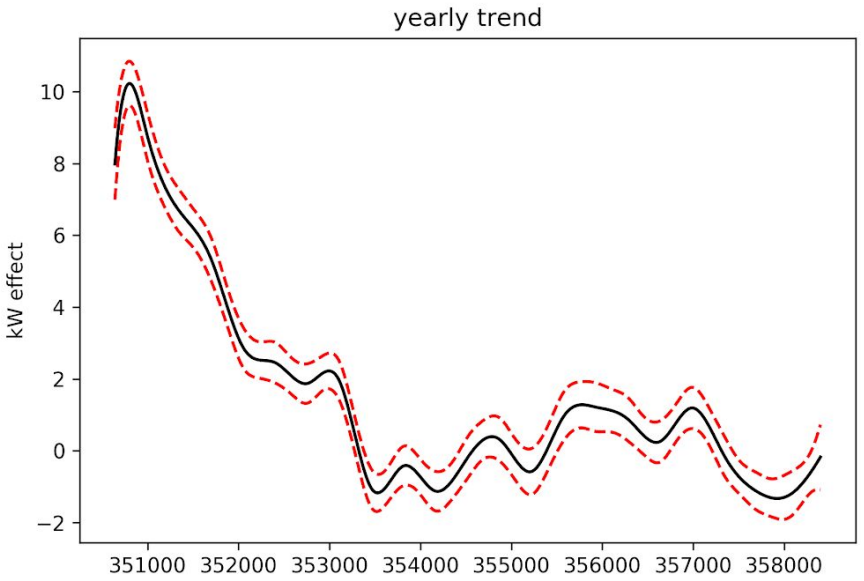


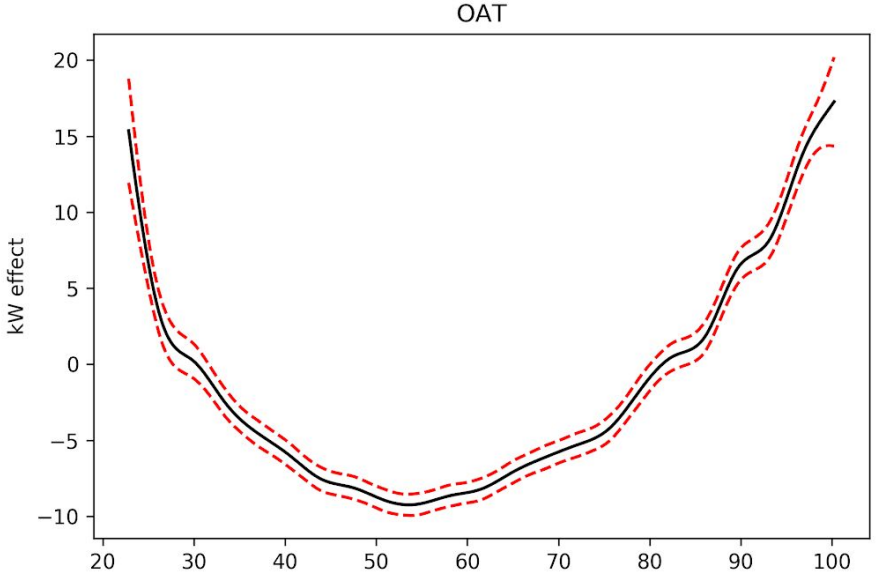
Welcome to PyDatatopolis

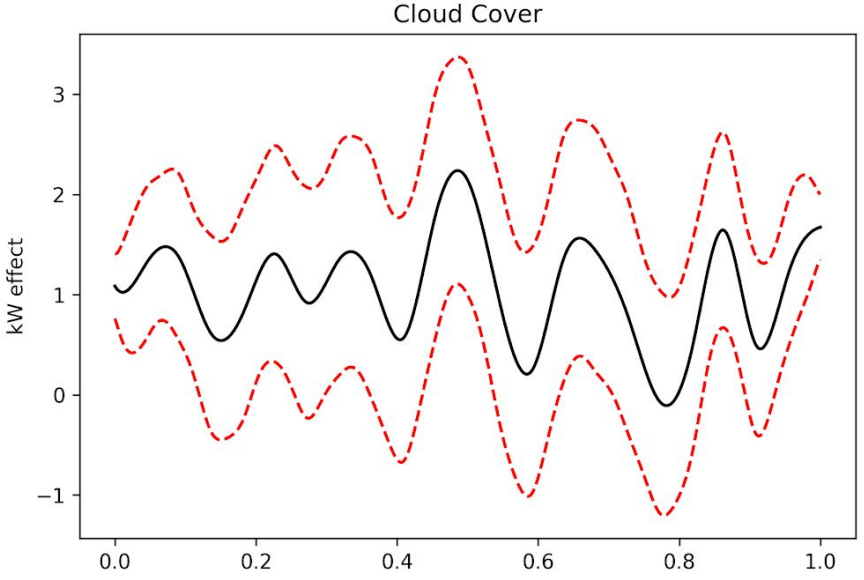
```
gam = LinearGAM(n_splines=[100, 25, 25, 25]).fit(X, y)
```

Welcome to PyDatatopolis





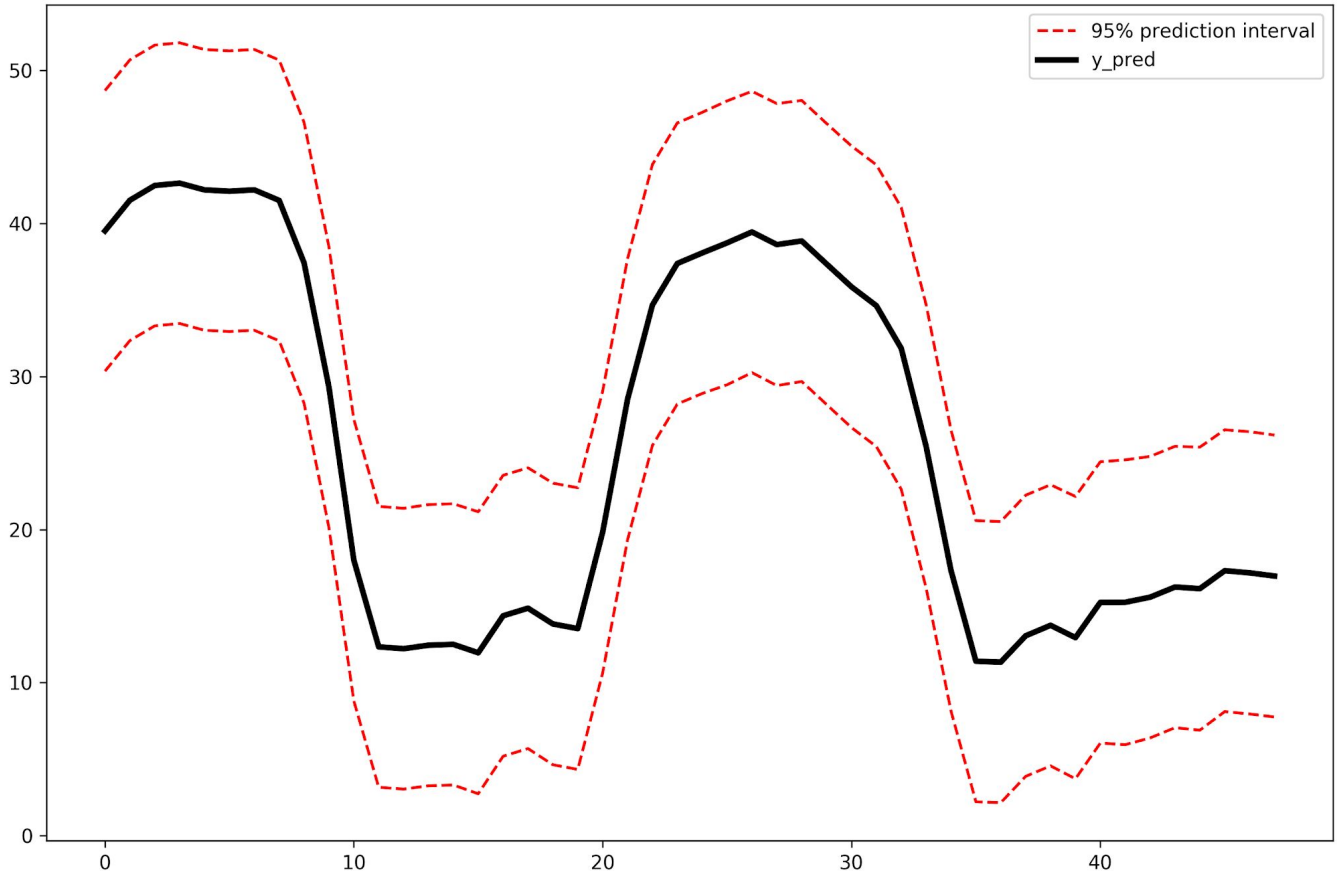




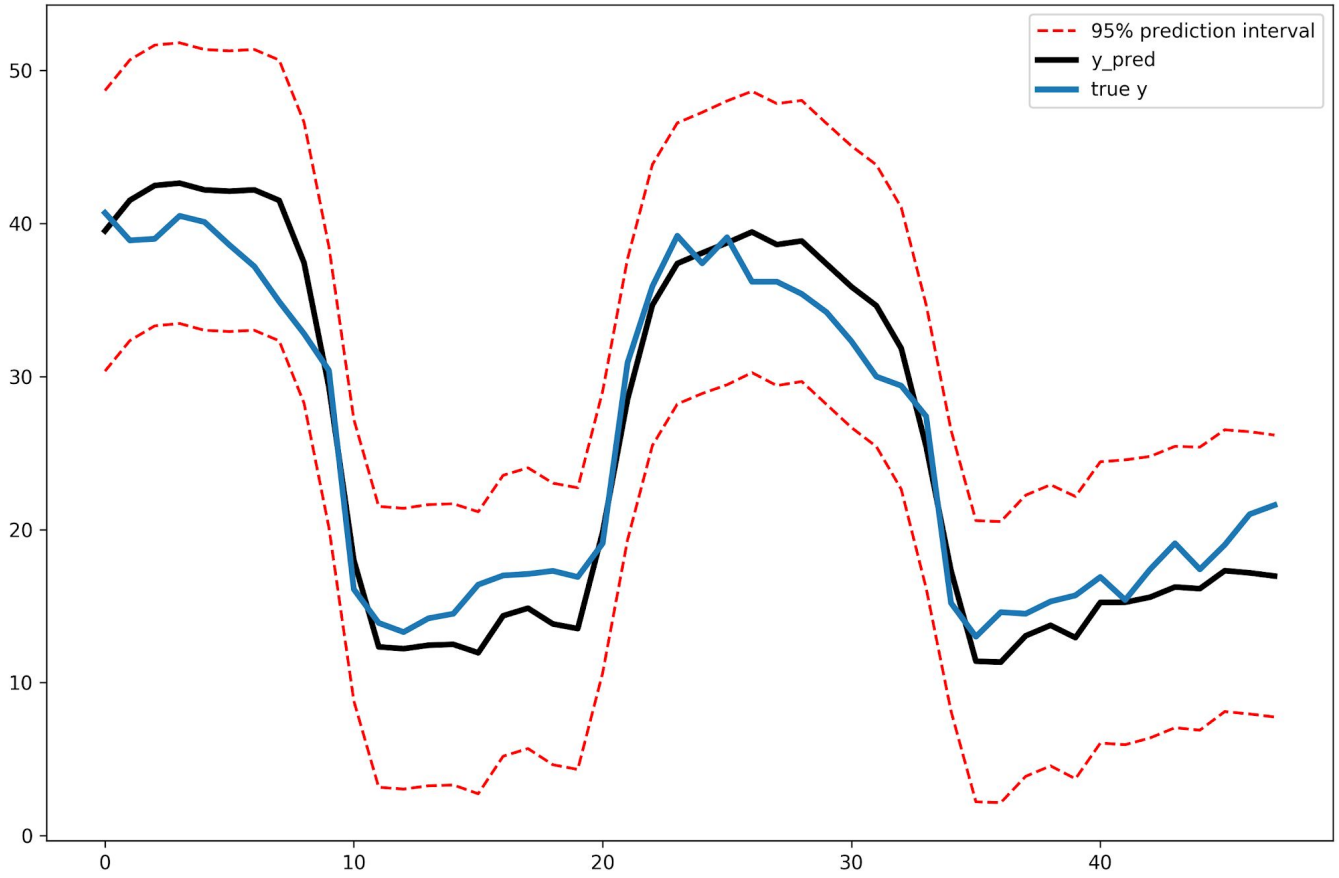
Welcome to PyDatatopolis

```
y_pred = gam.predict(X_pred)
predi = gam.prediction_intervals(X_pred, width=0.95)

plt.plot(predi, c='r', ls='--')
plt.plot(y_pred, c='k')
```

Welcome to PyDatatopolis



Welcome to PyDatatopolis



Welcome to PyDatatopolis

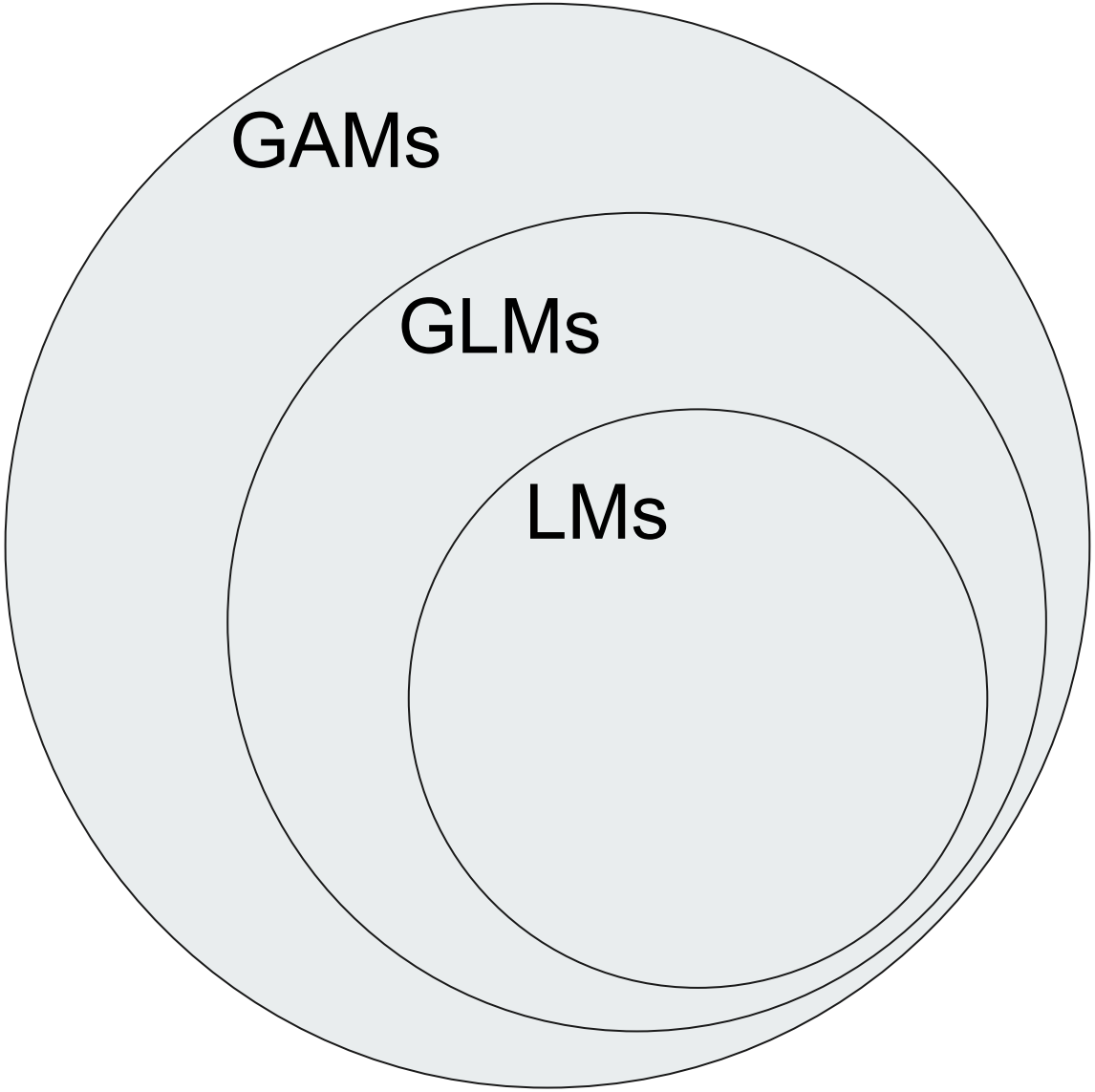
Open questions…

- How do we choose the smoothness?
- Feature selection?

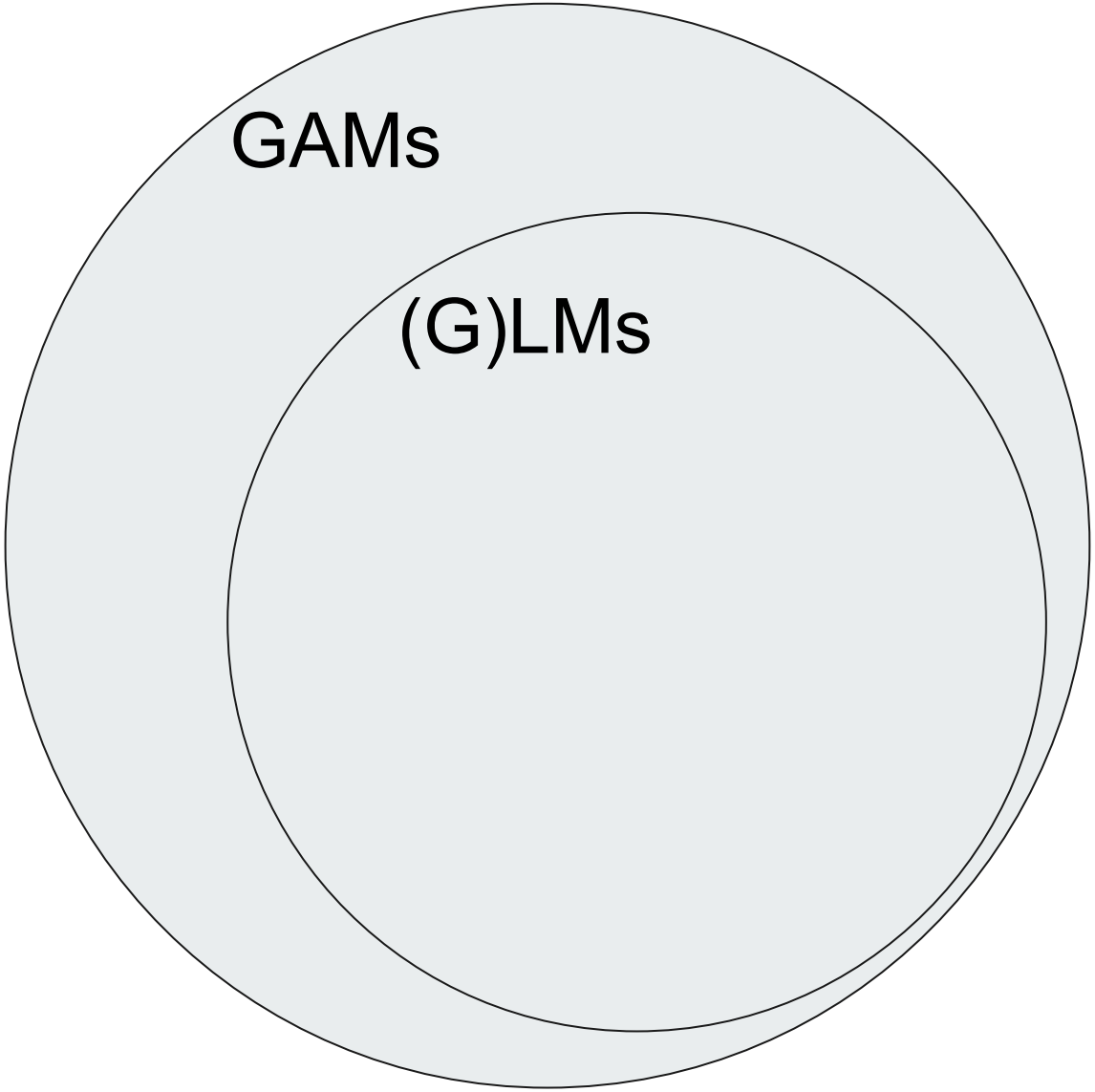
Plan

- What are GAMs
- A brief tour or splines
- Smoothing

What are GAMs

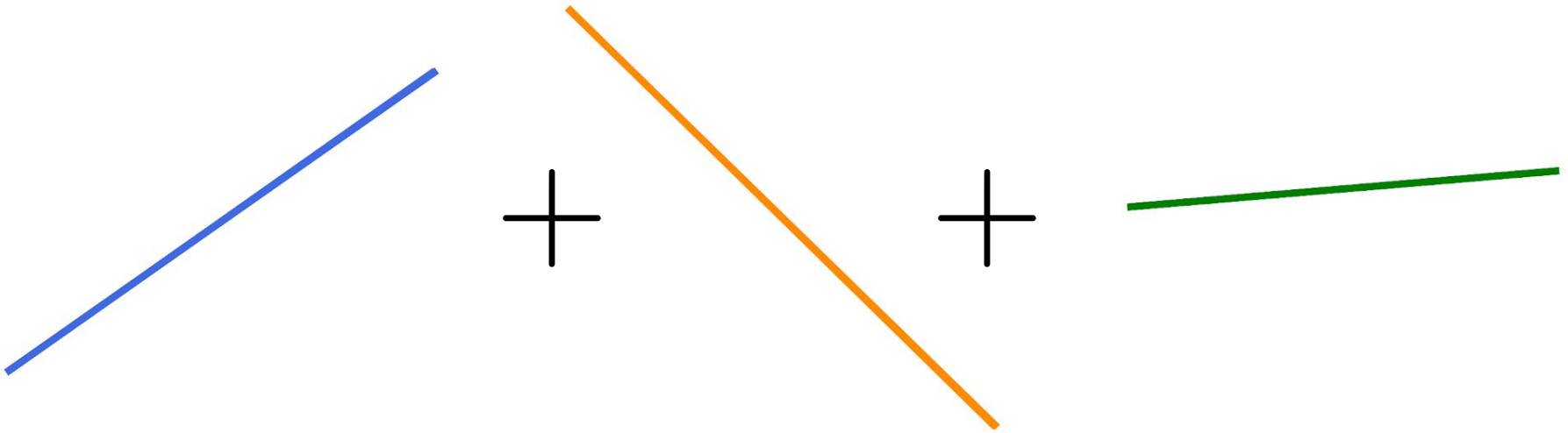


What are GAMs



What are GAMs

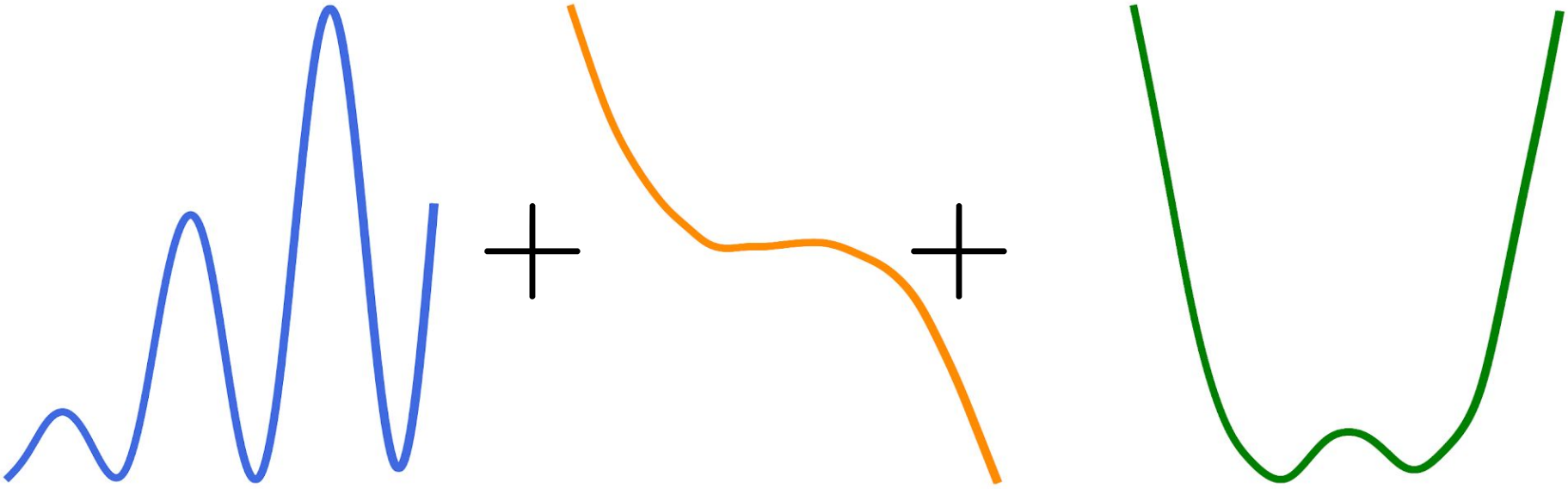
Linear Model



$$y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + c$$

What are GAMs

GAM



$$y = f_1(x_1) + f_2(x_2) + f_3(x_3) + c$$

What are GAMs

In general...

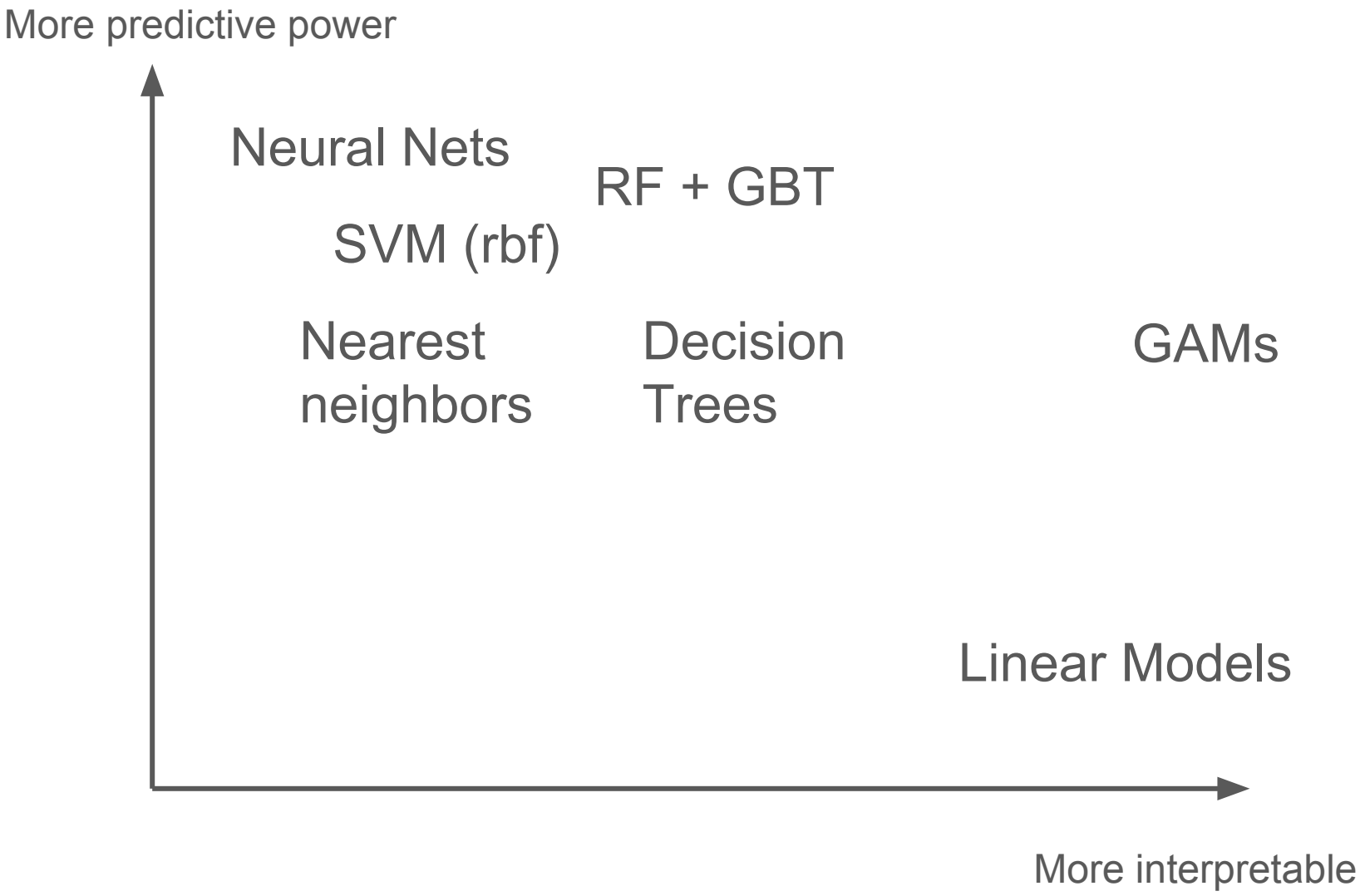
$$y = f_1(x_1) + f_2(x_2, x_3) + f_3(x_4) + \cdots + c$$

What are GAMs

but for us...

$$y = f_1(x_1) + f_2(x_2) + f_3(x_3) + c$$

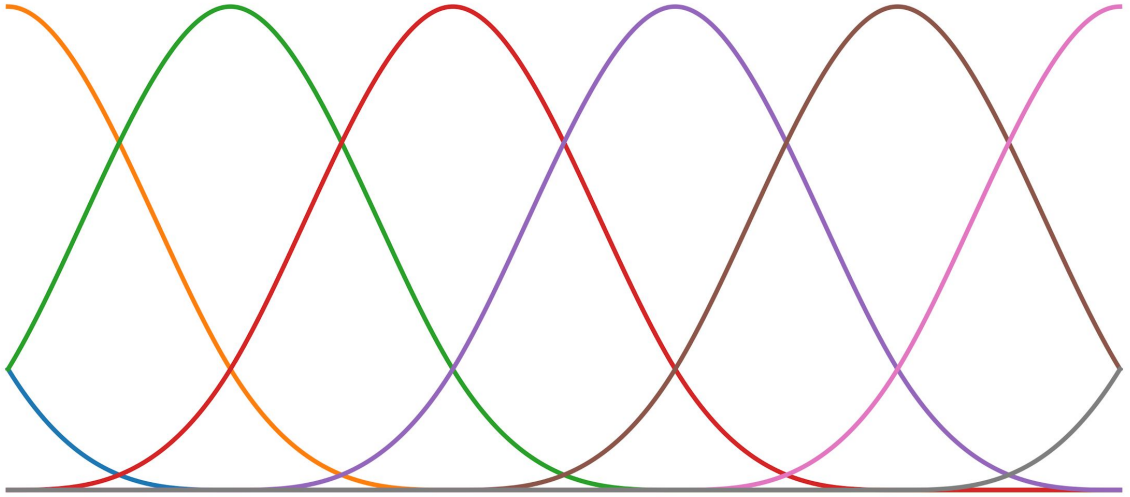
What are GAMs



What are GAMs

GAMs = GLMs

\+



\+ **Smoothing Penalty**

Plan

- What are GAMs
- A brief tour or splines
- Smoothing
- GAMs in Python

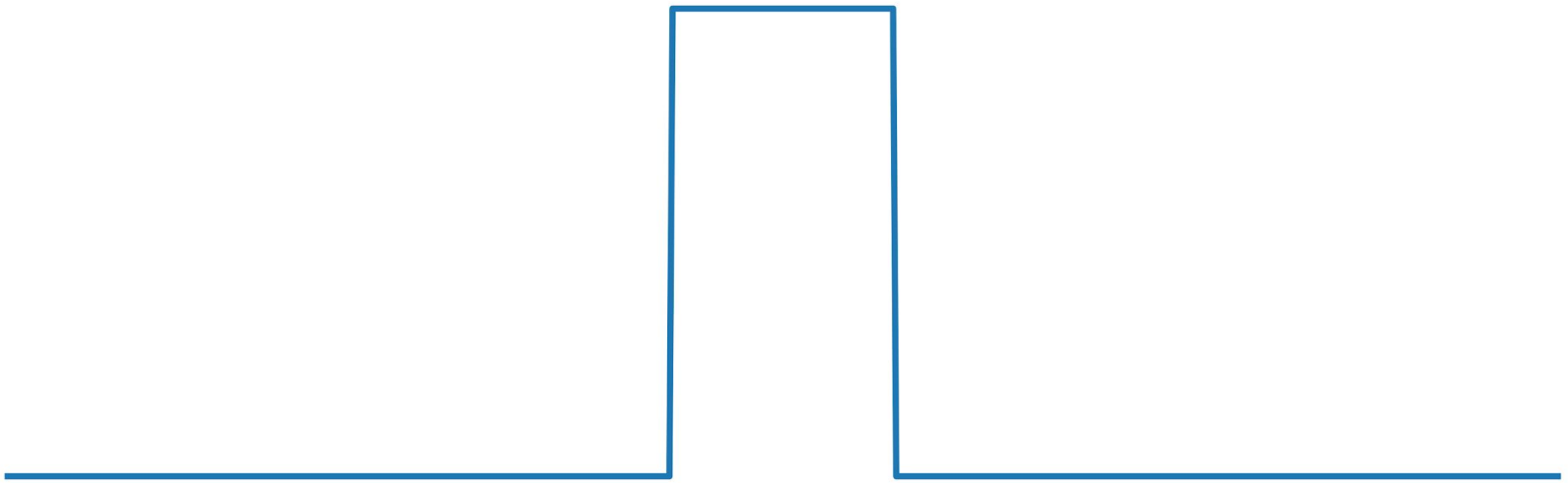
Splines

- Local support
- degree n spline has:
  - n + 1 segments of degree n
  - Continuous $(n-1)^{th}$ derivative

Splines

degree 0

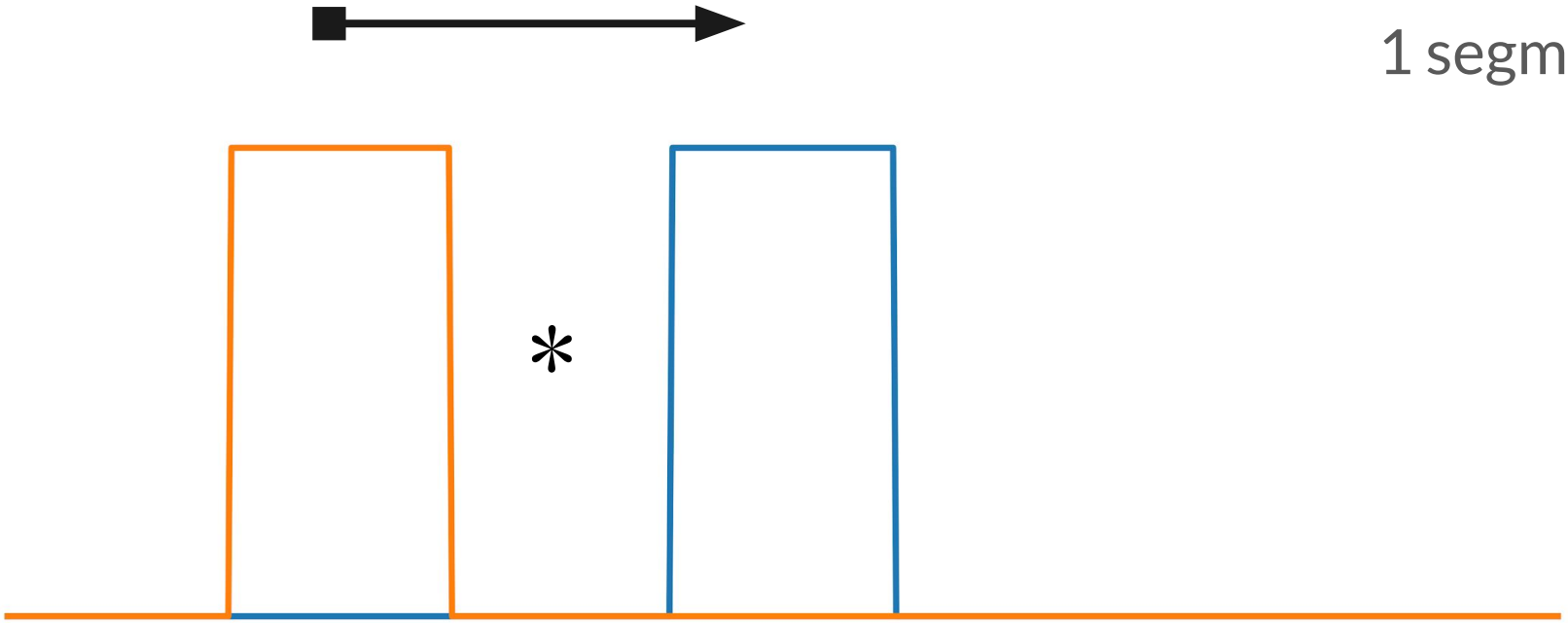
1 segment



Splines

degree 0

1 segment

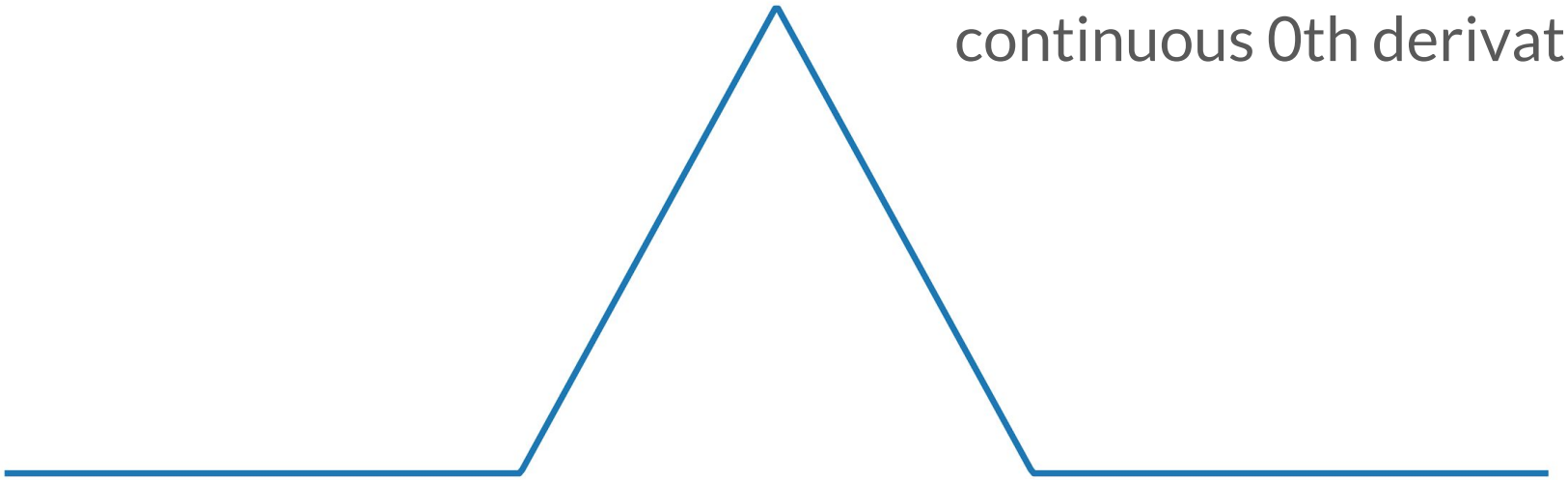


Splines

degree 1

2 segments

continuous 0th derivative

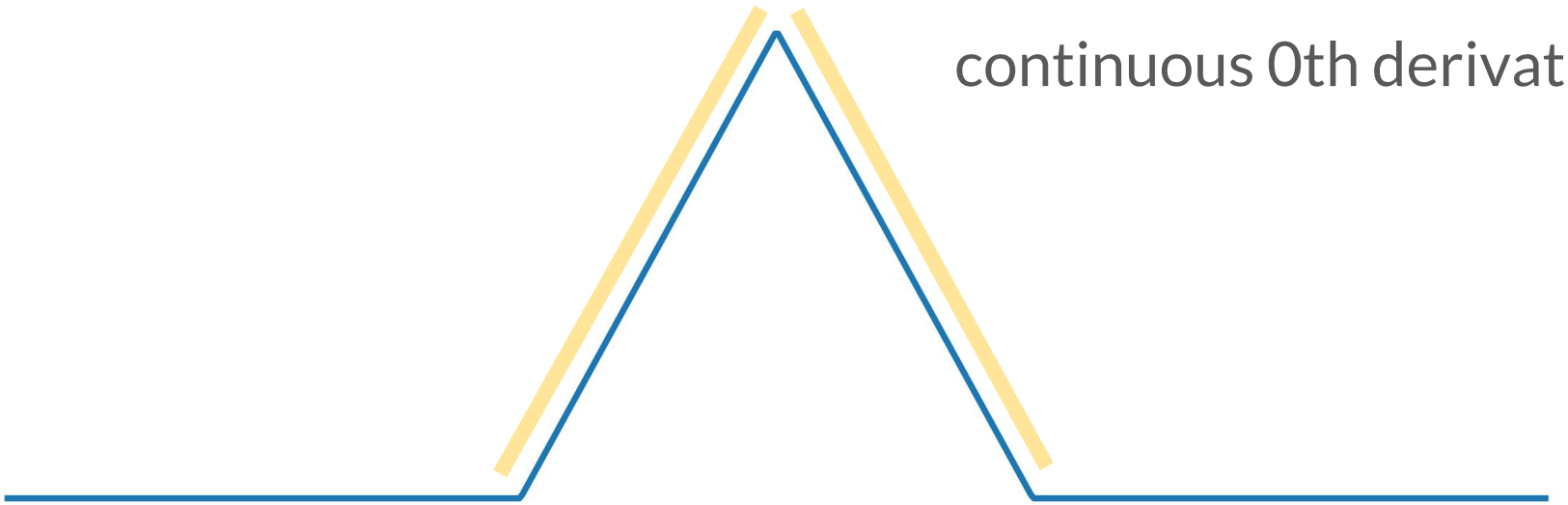


Splines

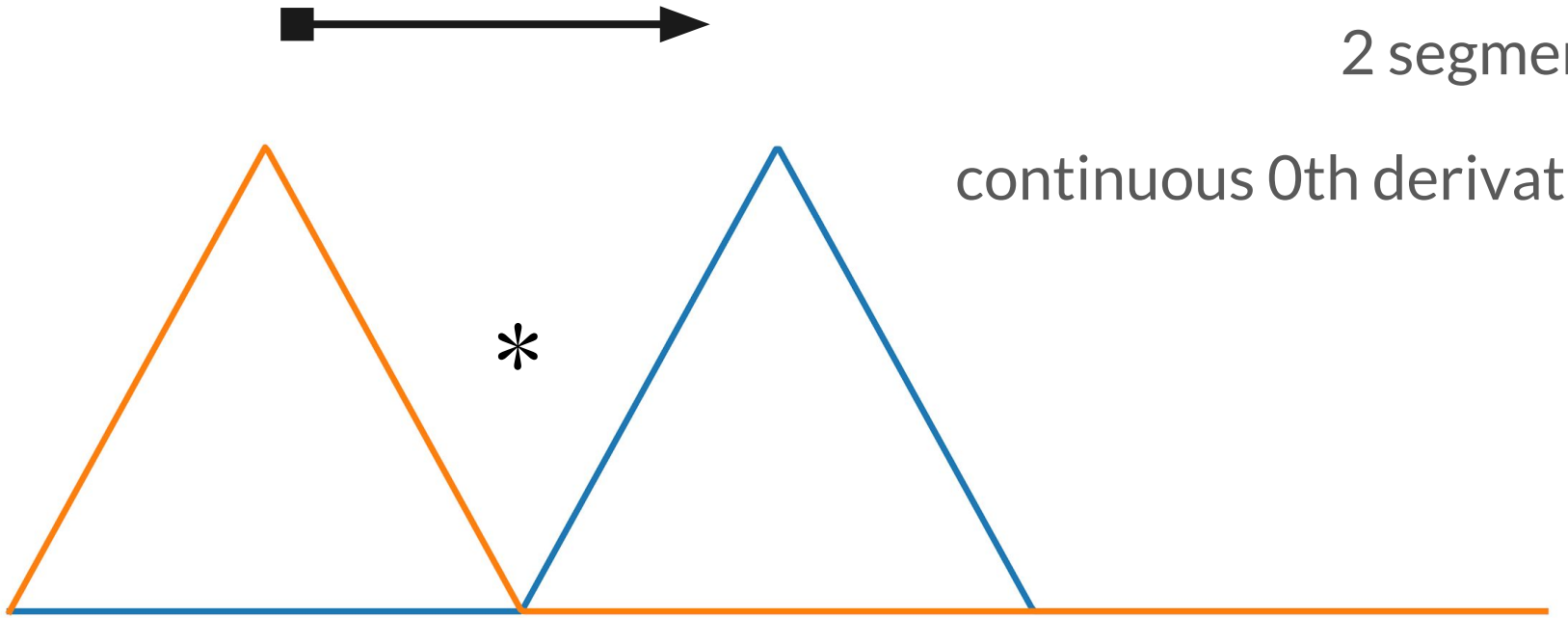
degree 1

2 segments

continuous 0th derivative



Splines



degree 1

2 segments

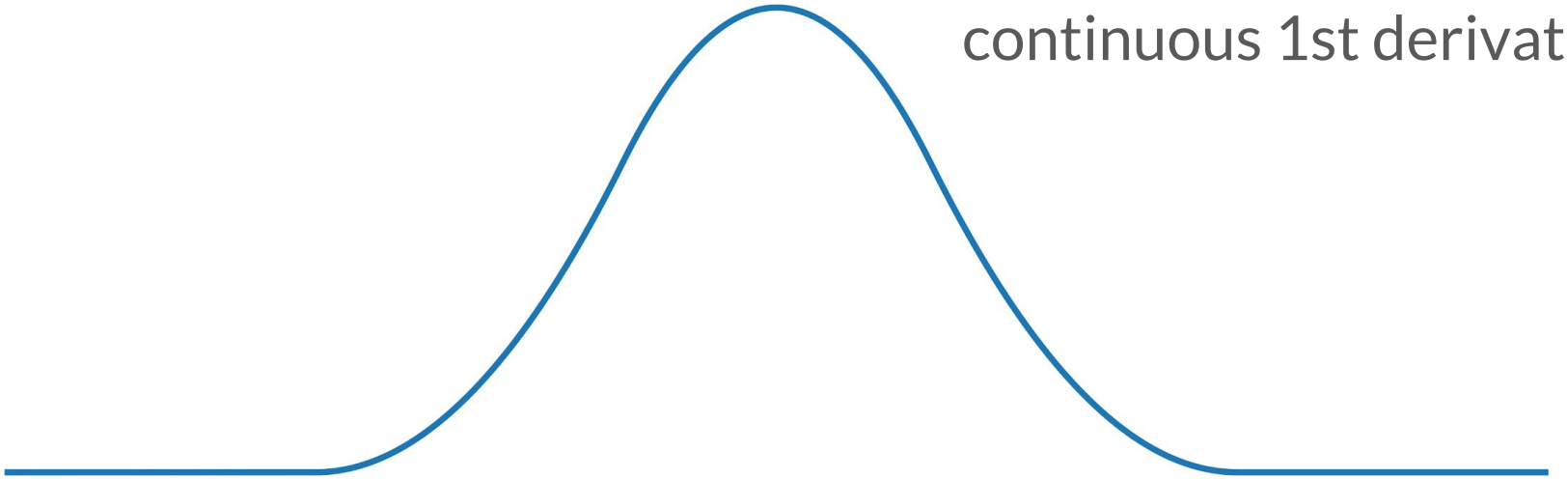
continuous 0th derivative

Splines

degree 2

3 segments

continuous 1st derivative

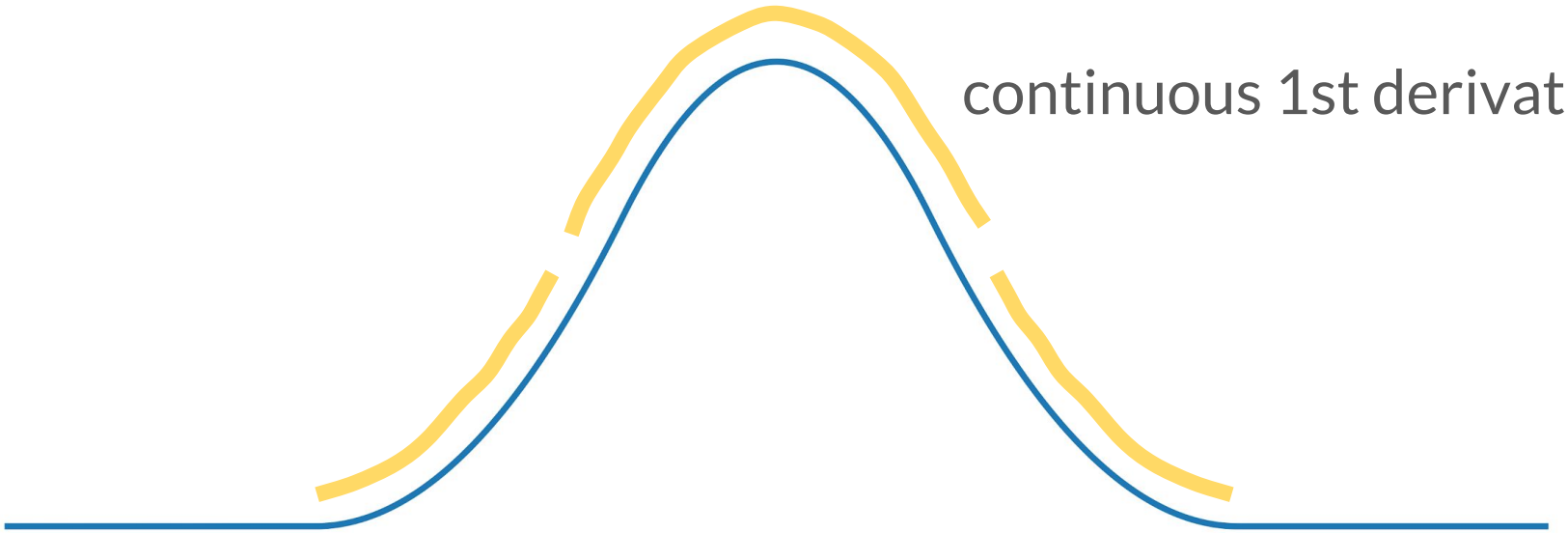


Splines

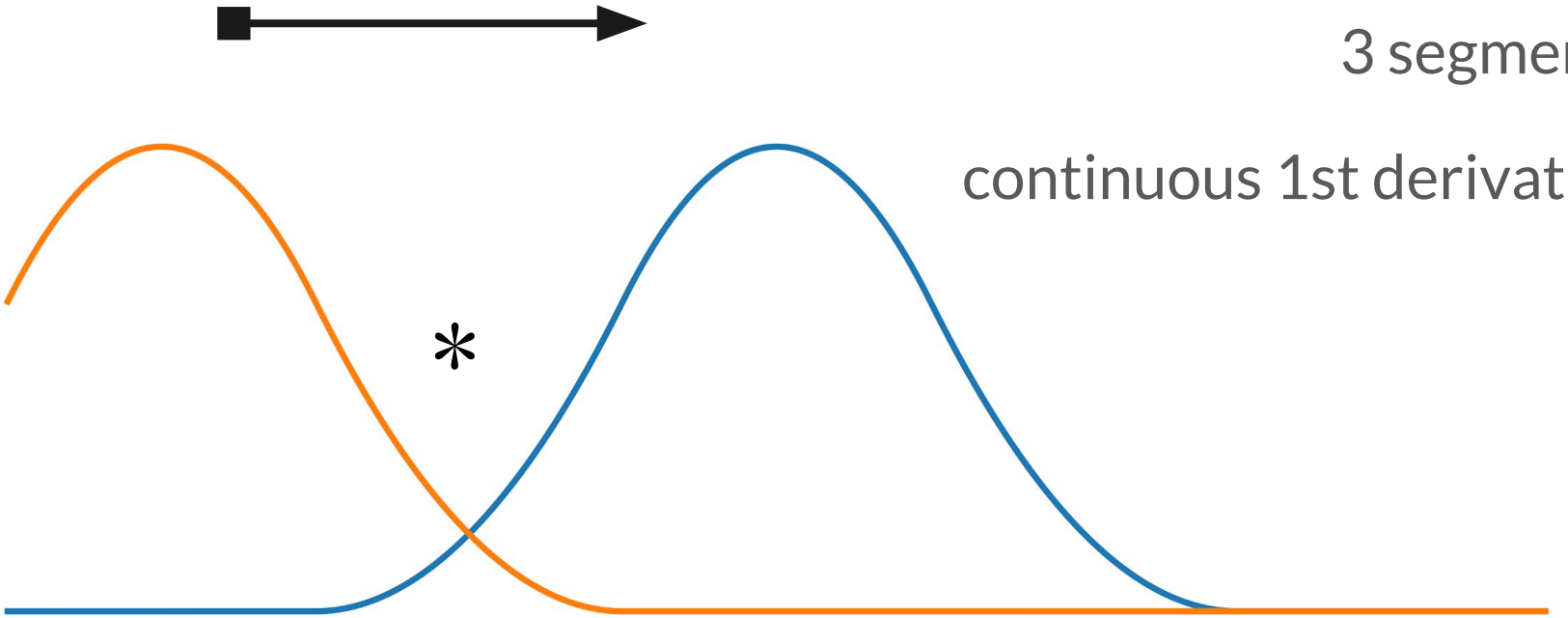
degree 2

3 segments

continuous 1st derivative



Splines



degree 2

3 segments

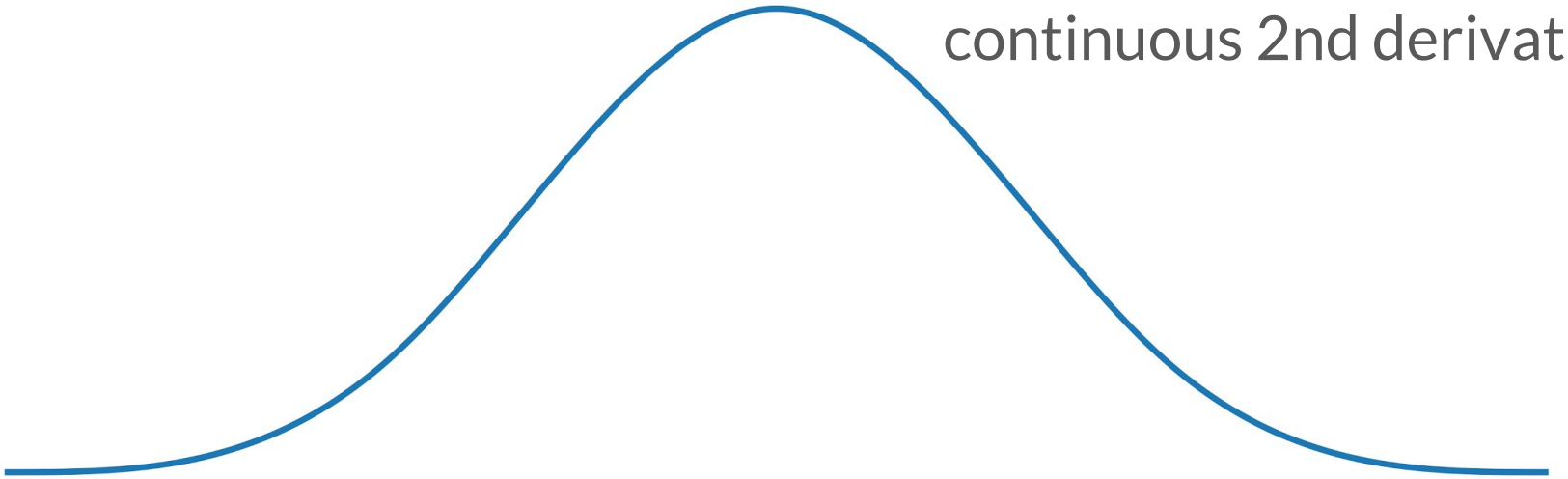
continuous 1st derivative

Splines

degree 3

4 segments

continuous 2nd derivative



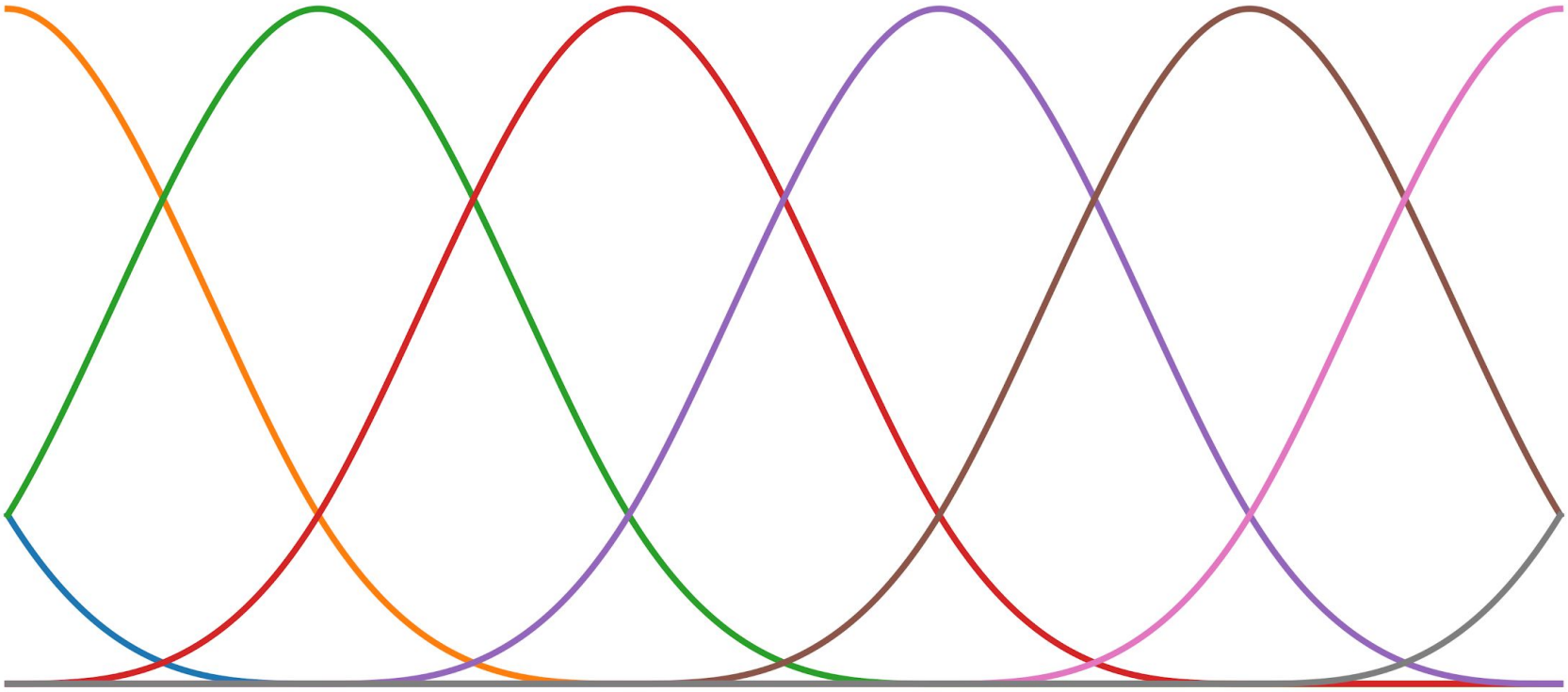
Splines

Spline -> Gaussian

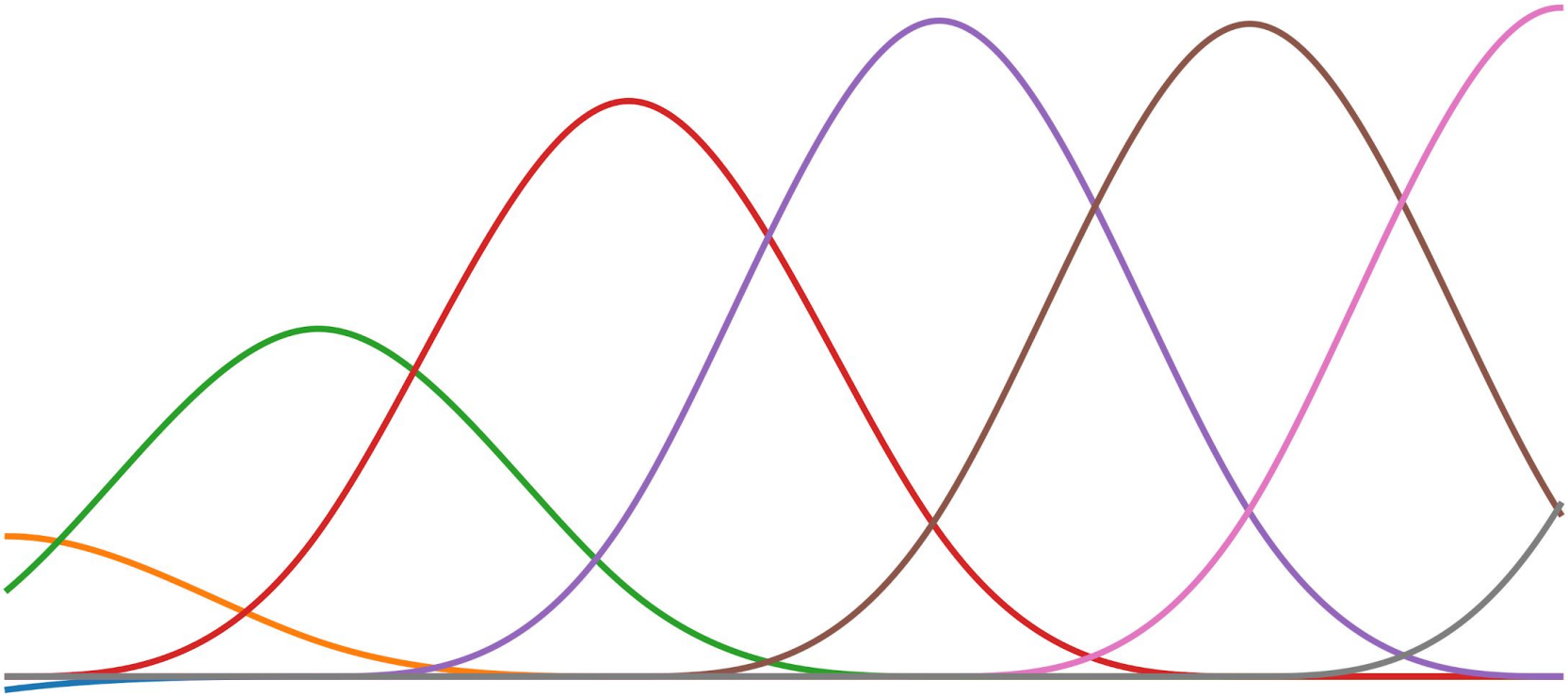
as

Spline Degree -> Infinity

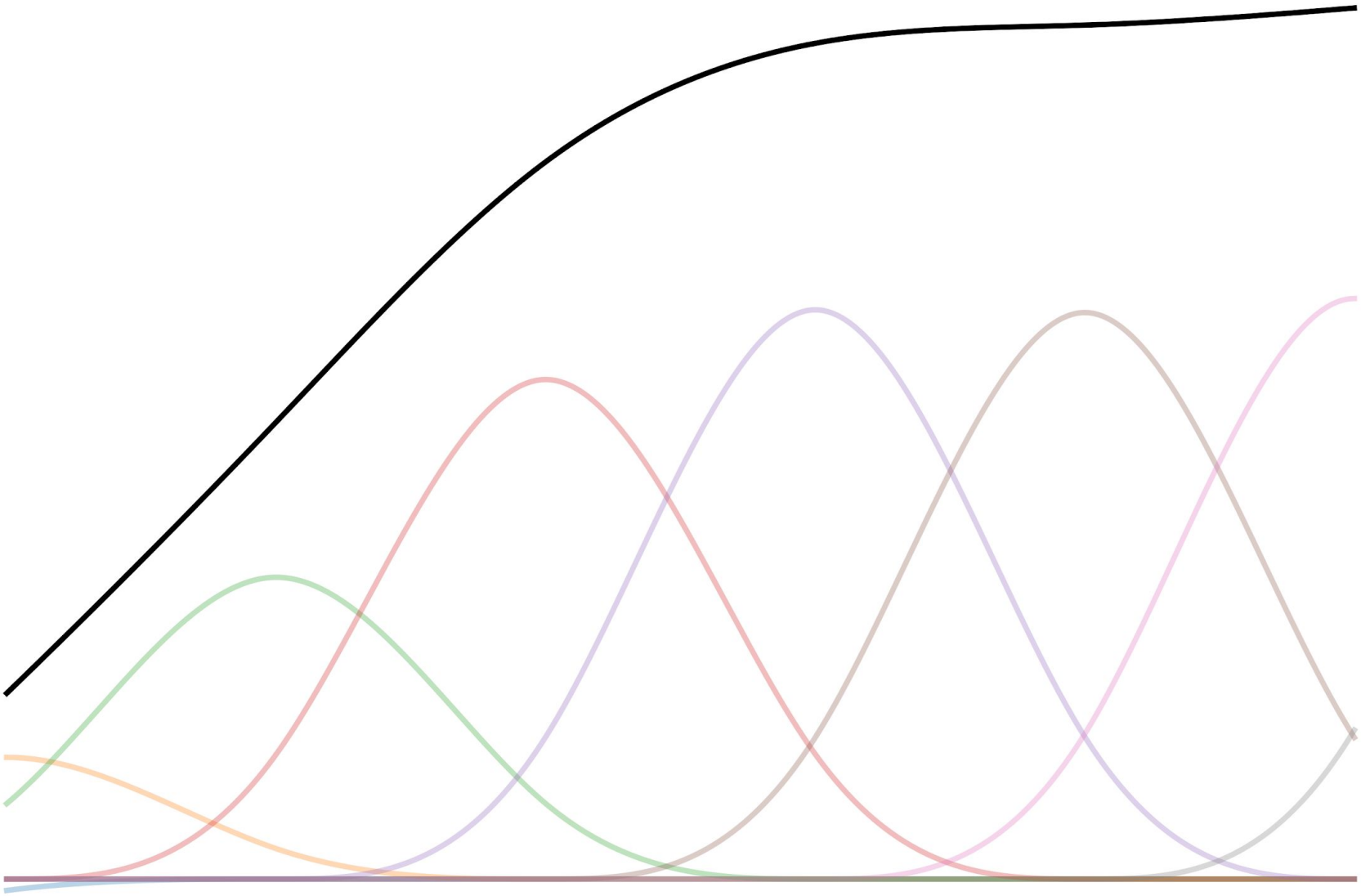
Splines



Splines



Splines



Some math...

A simple linear model:

$$y_i = X_i\beta + \epsilon_i$$

$$\epsilon_i = \mathcal{N}(0, \sigma^2)$$

Some math...

A simple GAM:

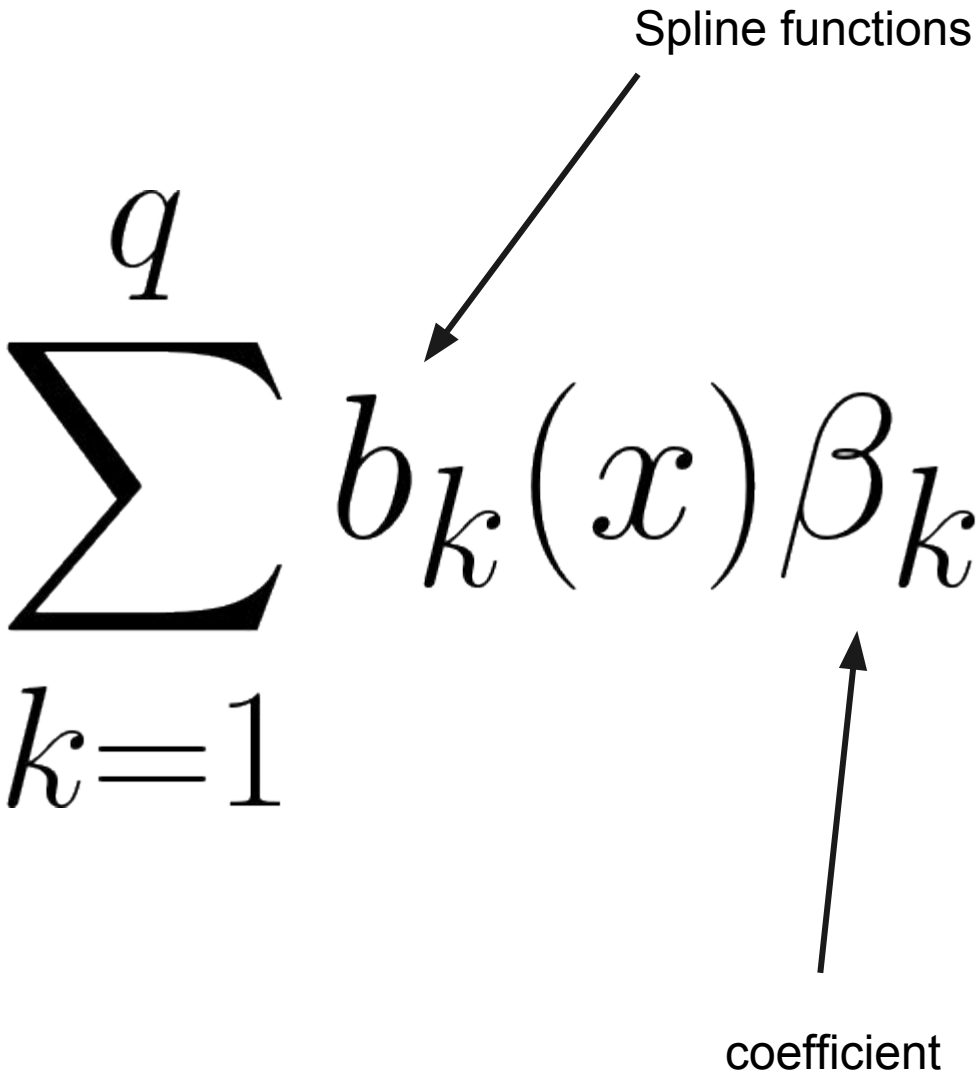
$$y_i = f(x_i) + \epsilon_i$$

$$\epsilon_i = \mathcal{N}(0, \sigma^2)$$

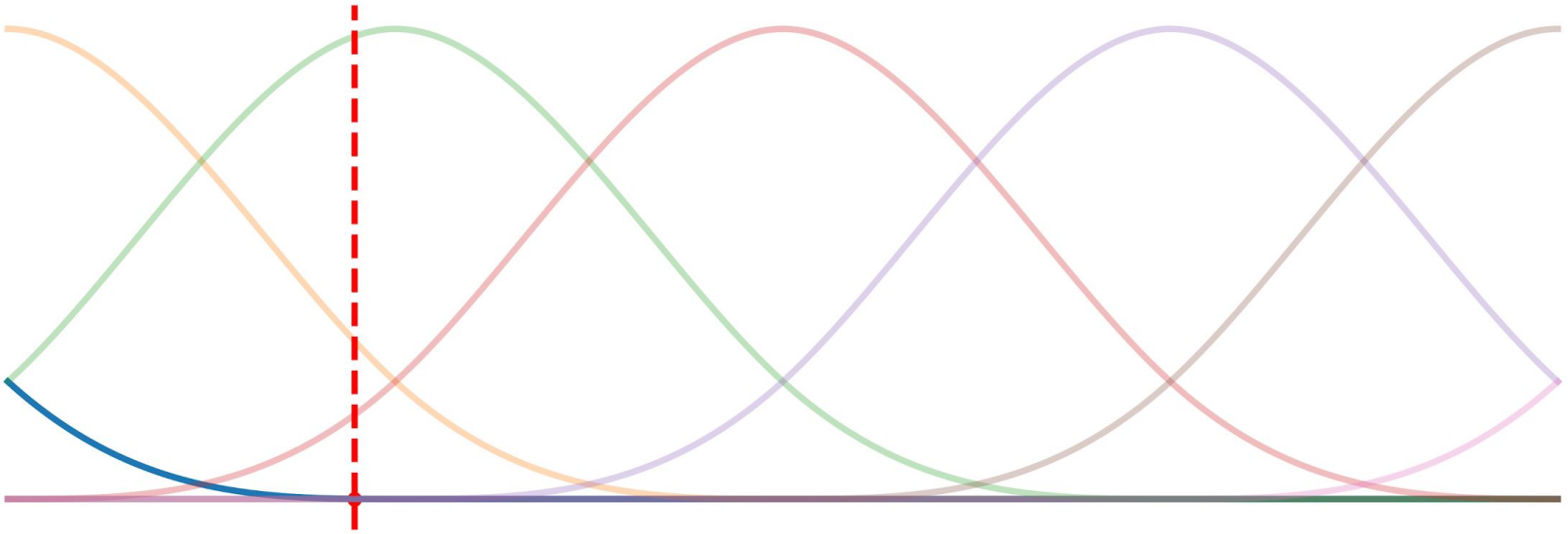
Some math...

$$f(x) = \sum_{k=1}^{q} b_k(x)\beta_k$$

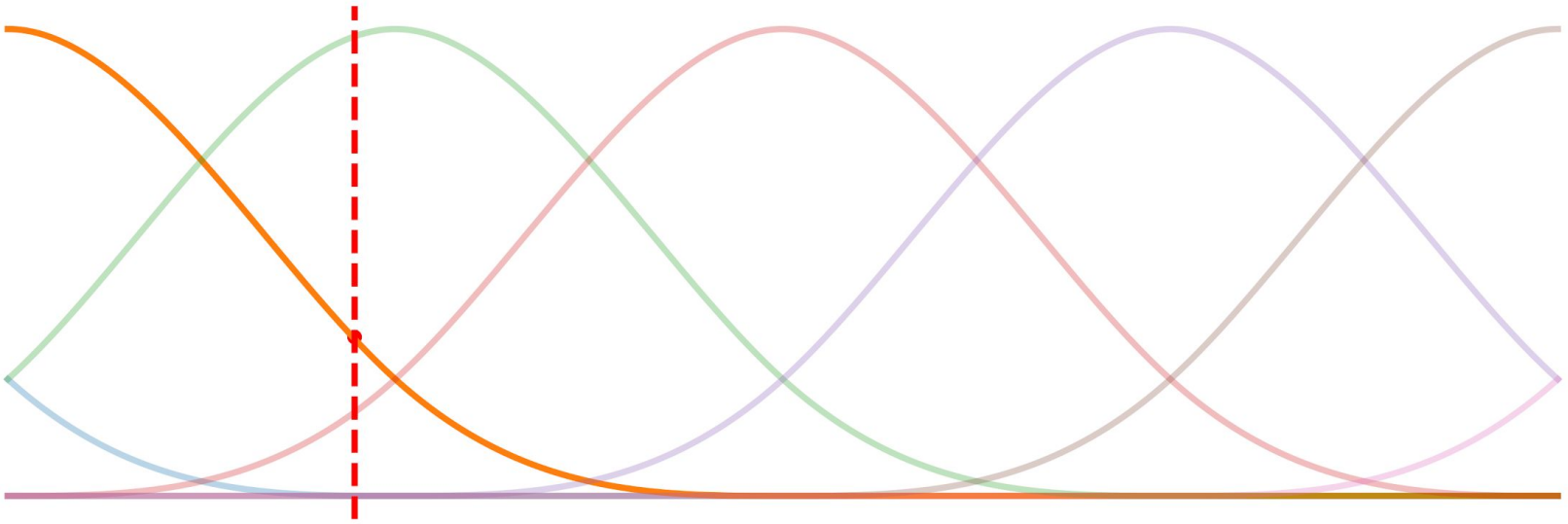
Some math...



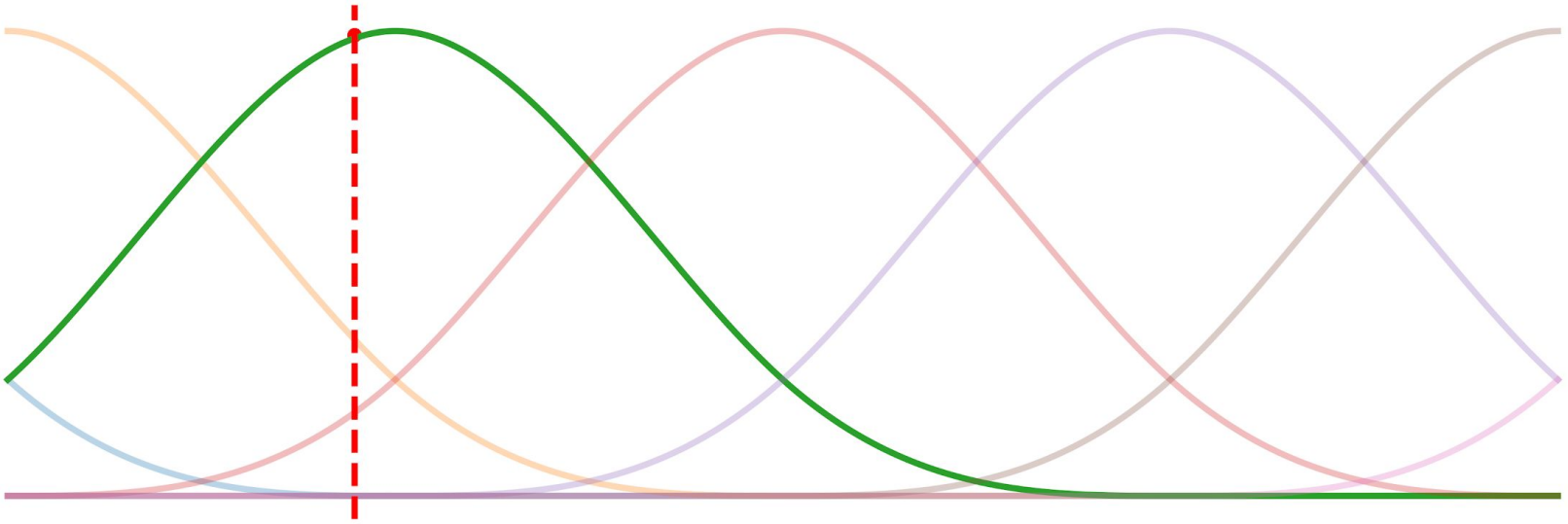
Some math...



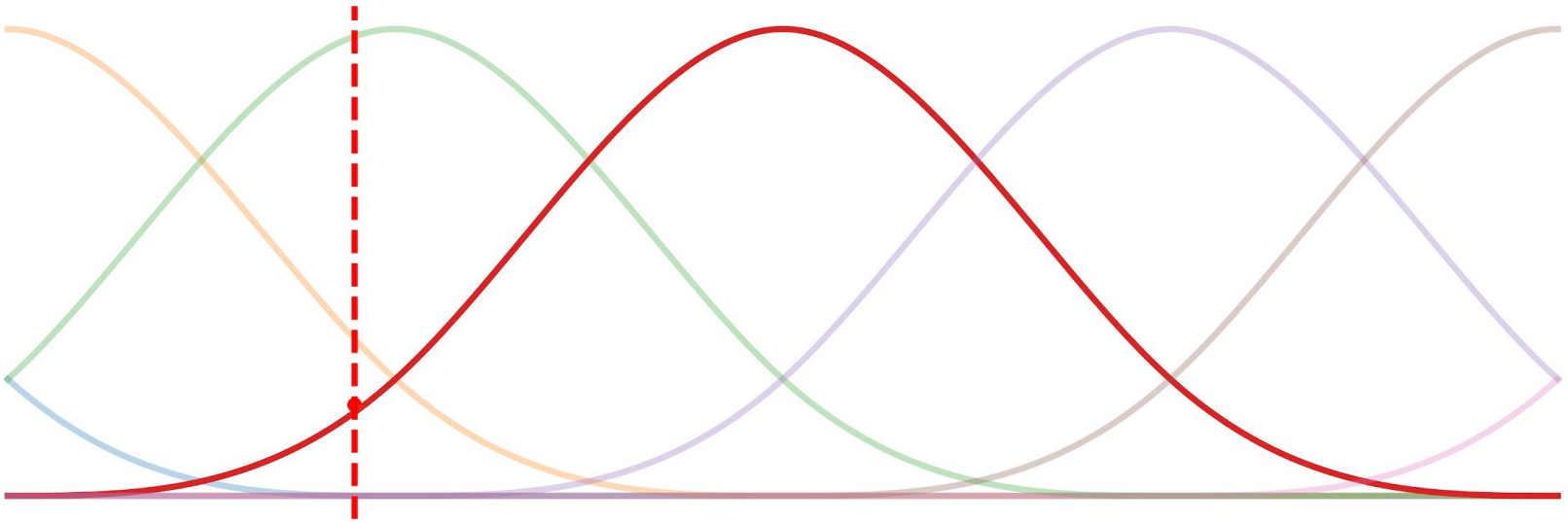
Some math...



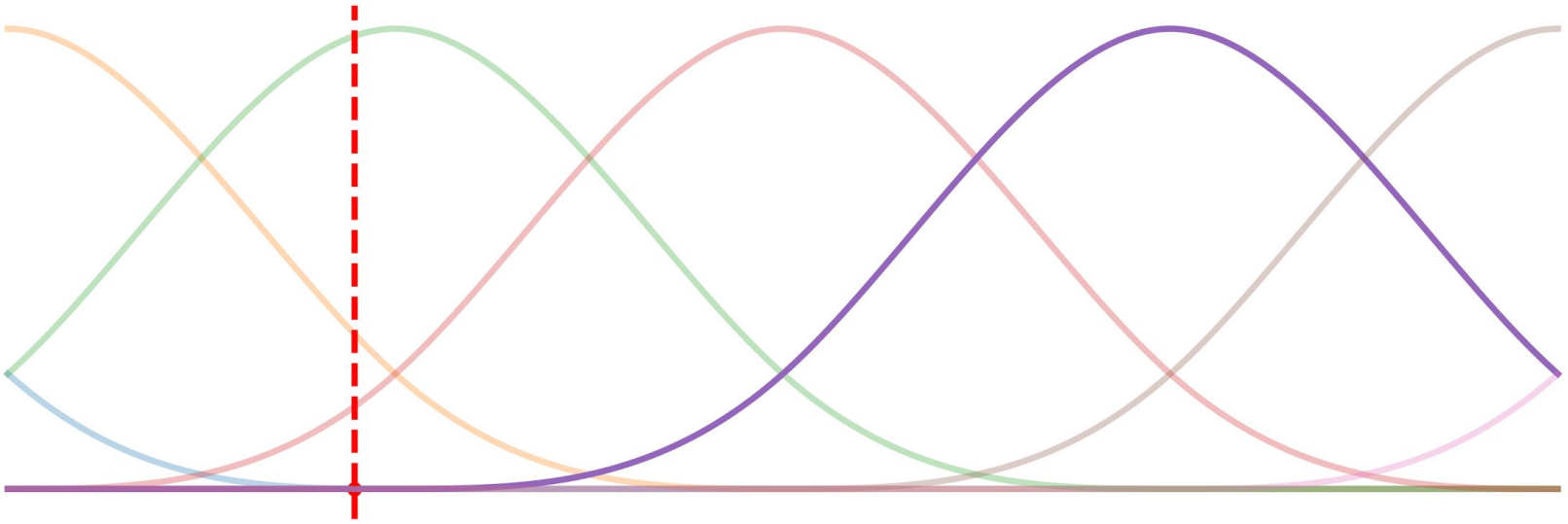
Some math...



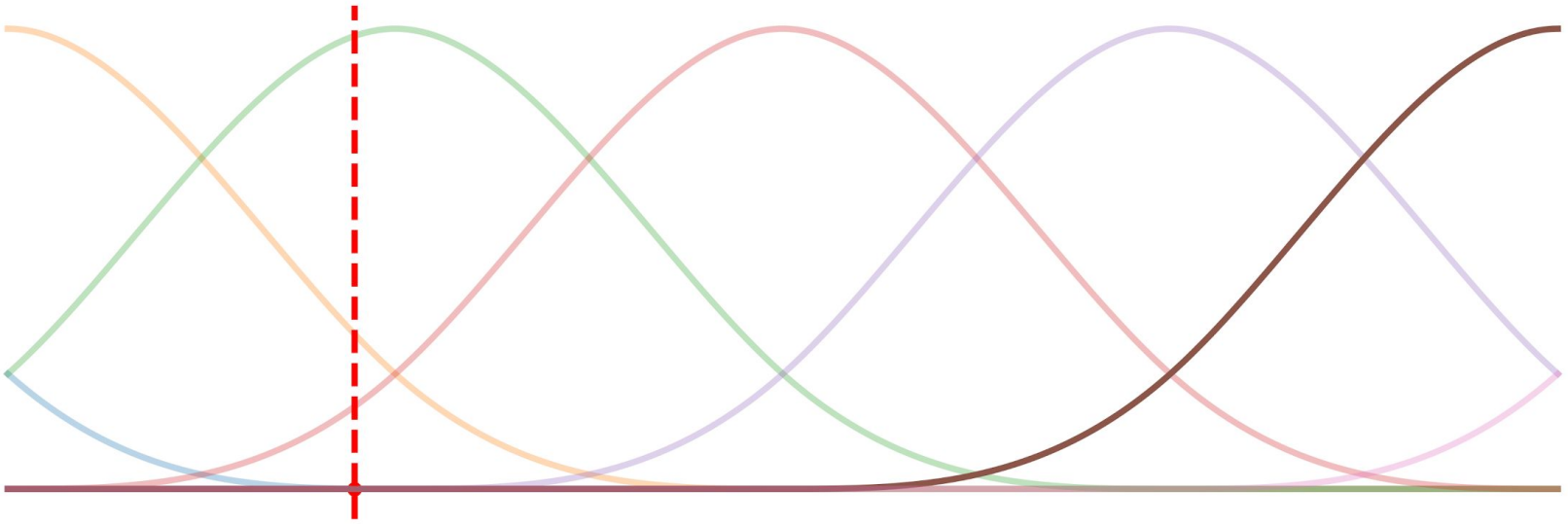
Some math...



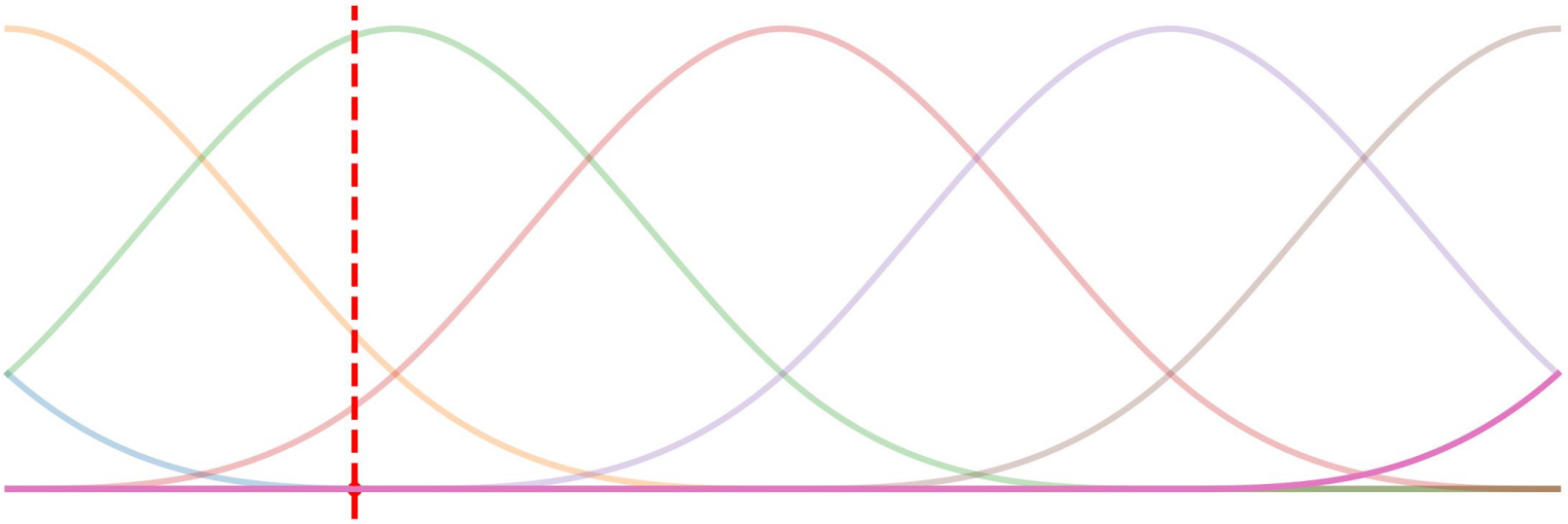
Some math...



Some math...



Some math...



Some math...

$$\sum_{k=1}^{q} b_k(x)\beta_k$$

Some math...

$$\sum_{k=1}^{q} \hat{x}_k \beta_k$$

Some math...

$$\hat{X}\beta$$

Some math...

$$y = \hat{X}\beta + \epsilon$$

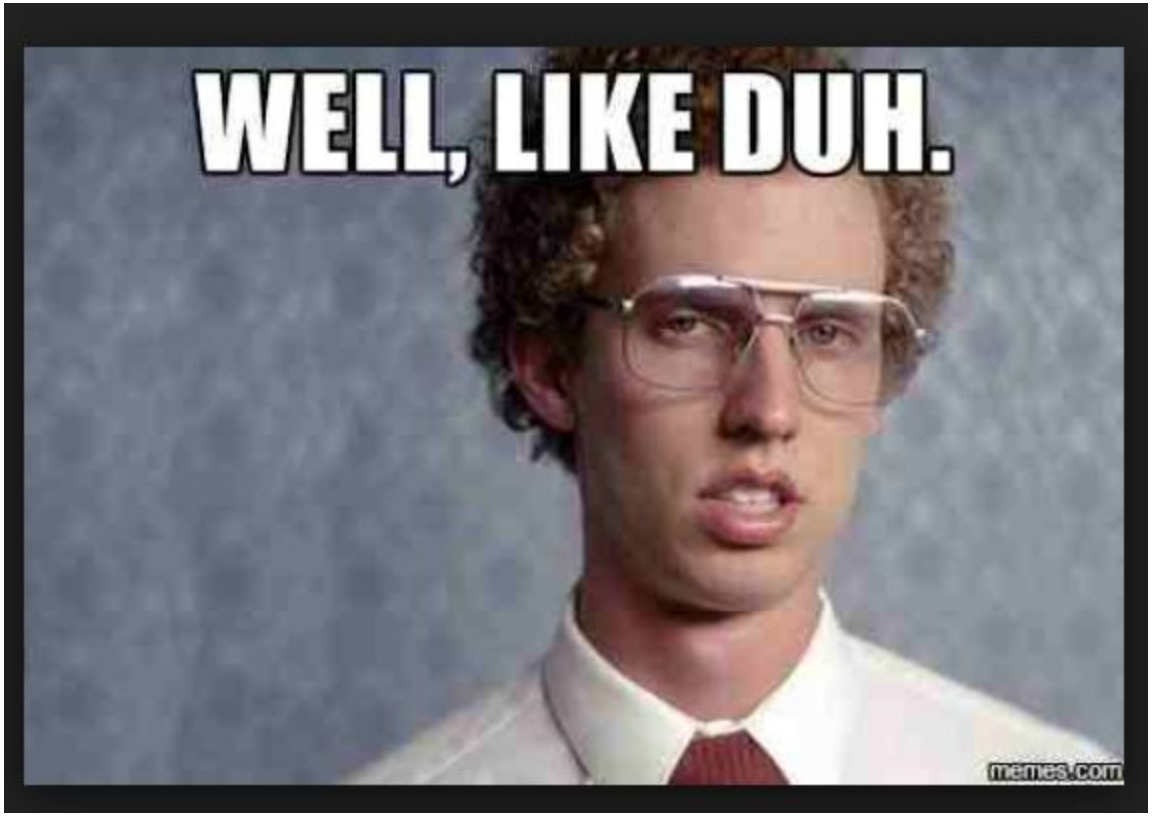
Some math...

$$y_i = \hat{X}_i \beta + \epsilon_i$$

Some math...

GAM = big GLM

Some math...

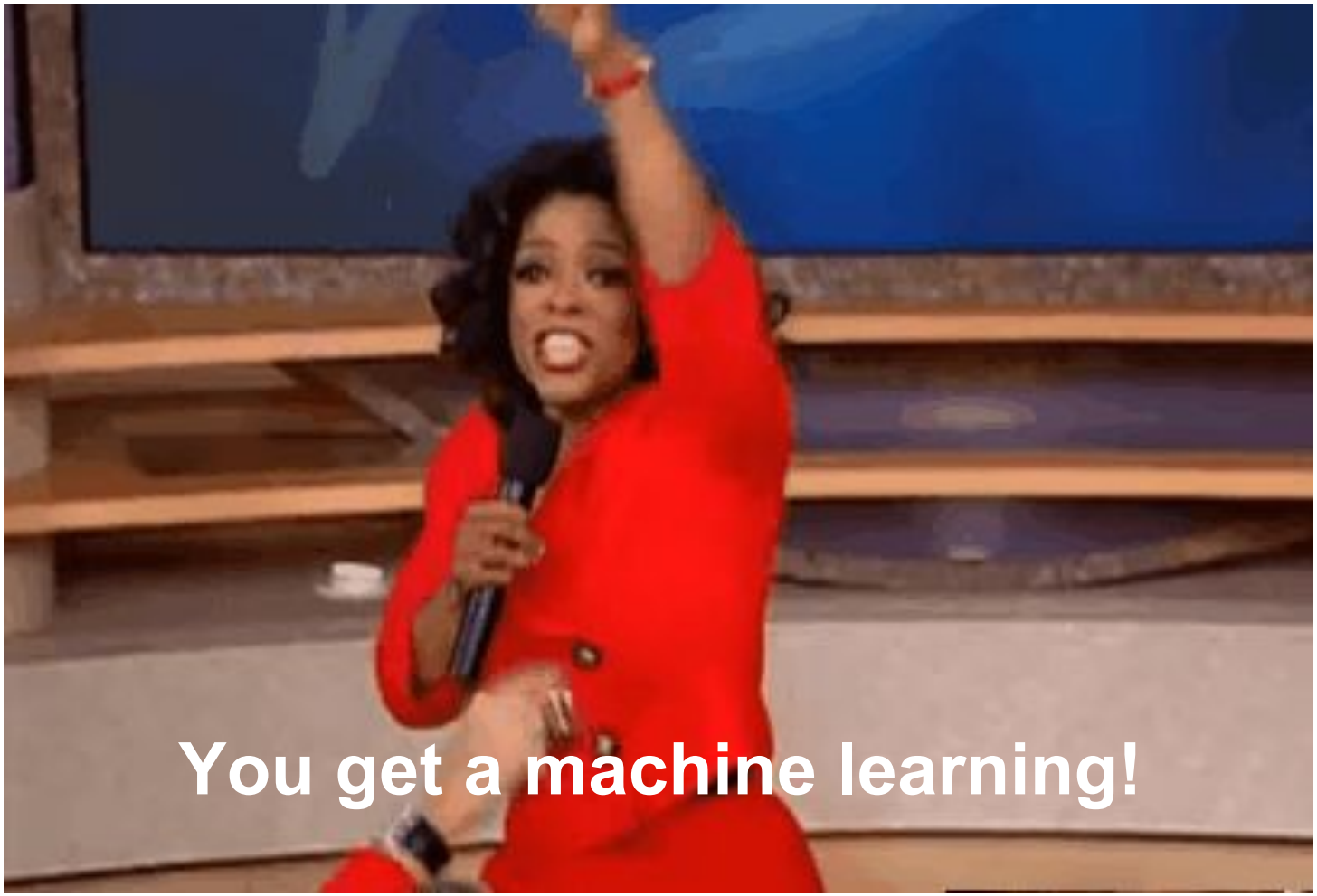


Free stuff!

Lots of **GLM** theory for free

- Confidence intervals
- Prediction intervals
- non-Normal observations
- Feature selection with p-values
- Fast cross-validation via GCV

Free stuff!

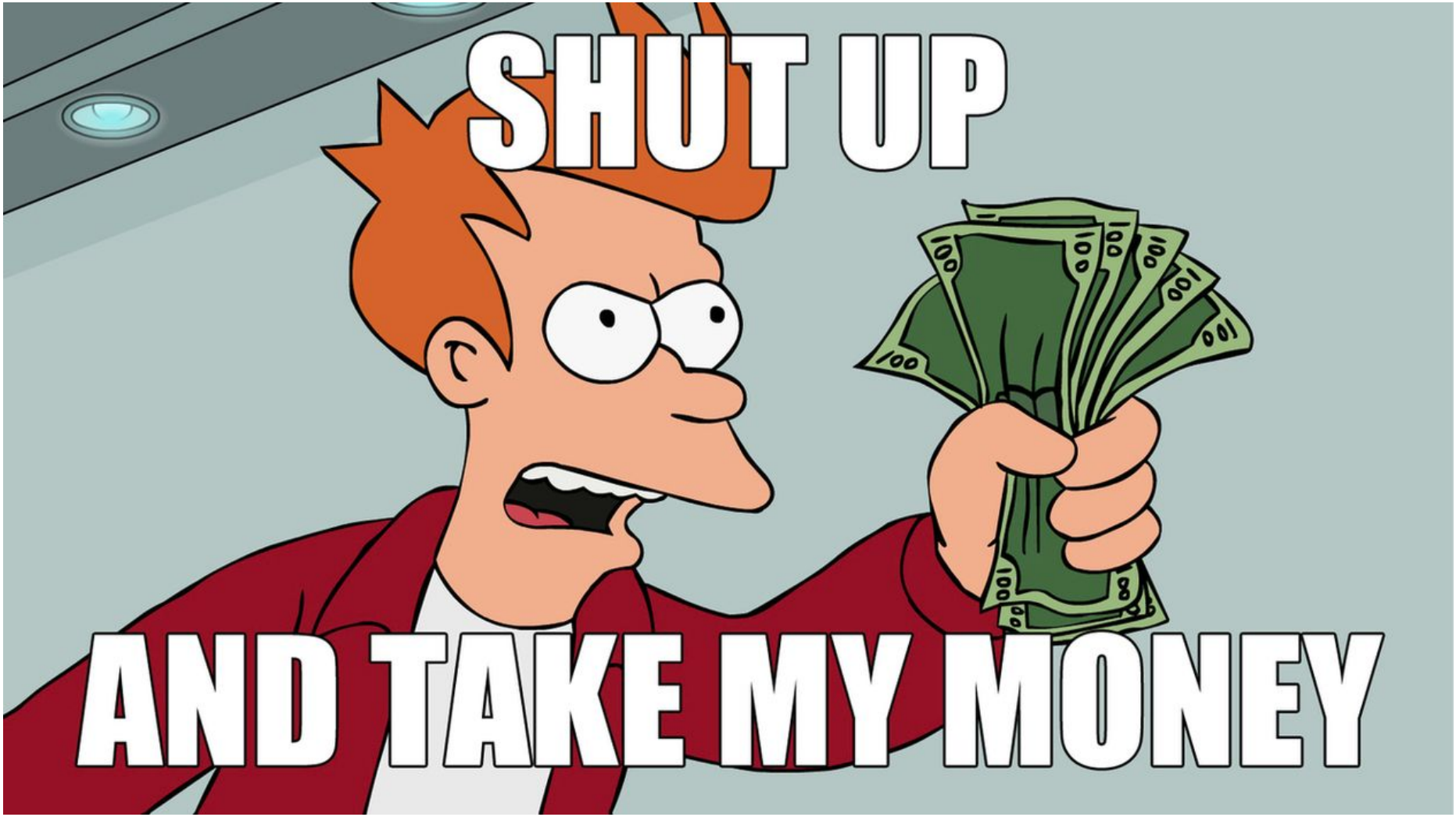


Free stuff!

And specific **GAM** stuff

- Intuitive regularization via smoothing
- Automatically model non-linearities
- Constraints (convexity, monotonicity, periodicity, ...)
- Controlled extrapolation

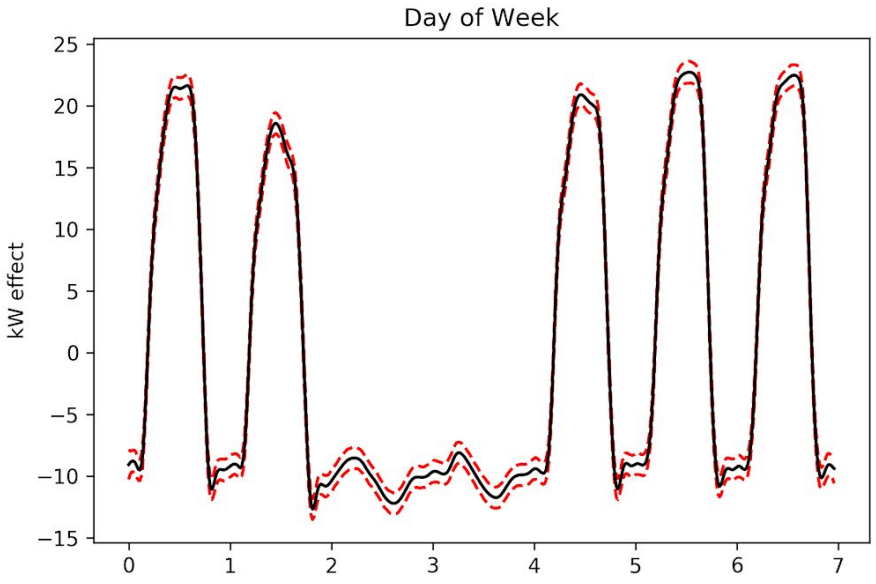
Free stuff!

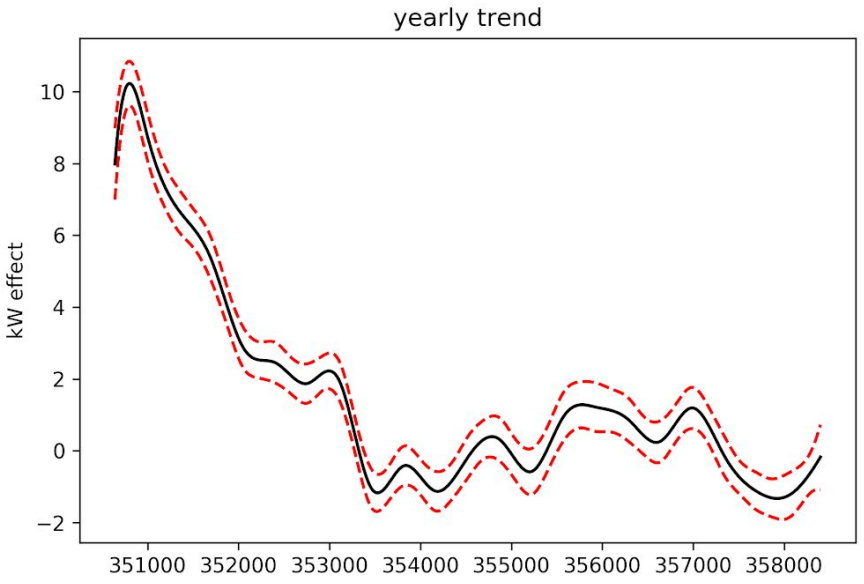


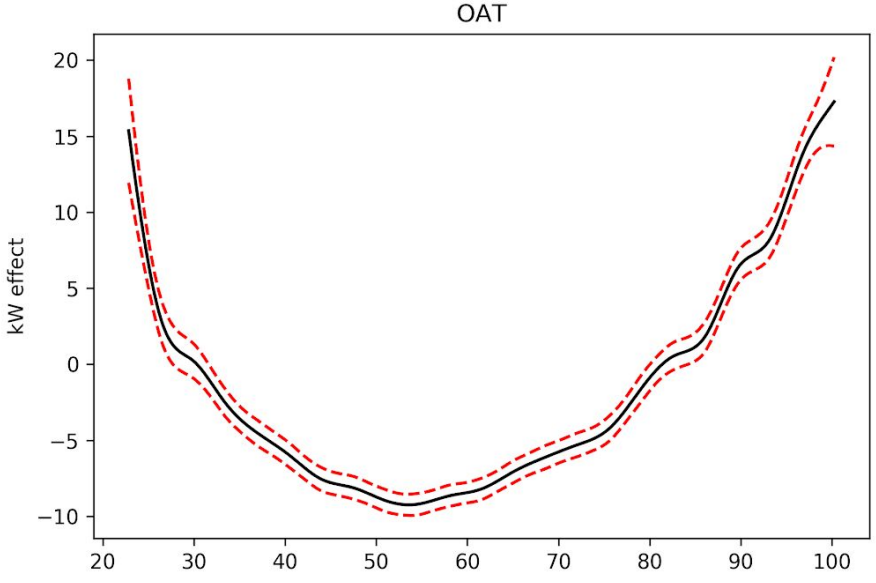
Plan

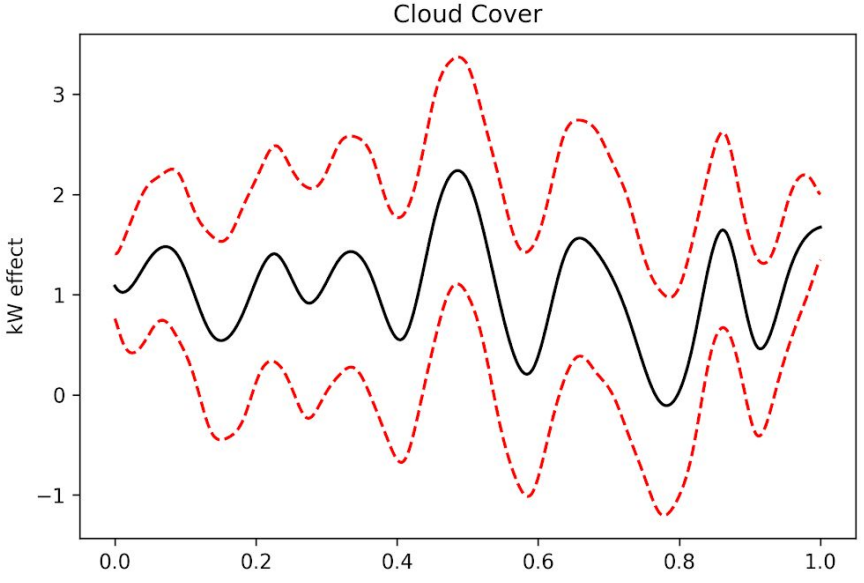
- What are GAMs
- A brief tour or splines
- Smoothing

Smoothing


Day of Week
kW effect
25
20
15
10
5
0
−5
−10
−15
0
1
2
3
4
5
6
7


yearly trend
kW effect
10
8
6
4
2
0
−2
351000
352000
353000
354000
355000
356000
357000
358000


OAT
kW effect
20
15
10
5
0
−5
−10
20
30
40
50
60
70
80
90
100


Cloud Cover
kW effect
3
2
1
0
−1
0.0
0.2
0.4
0.6
0.8
1.0

Smoothing

Penalize excessive wiggliness

$$wiggliness = \int_a^b [f''(x)]^2 dx$$

Smoothing

strength of smoothing

minimize

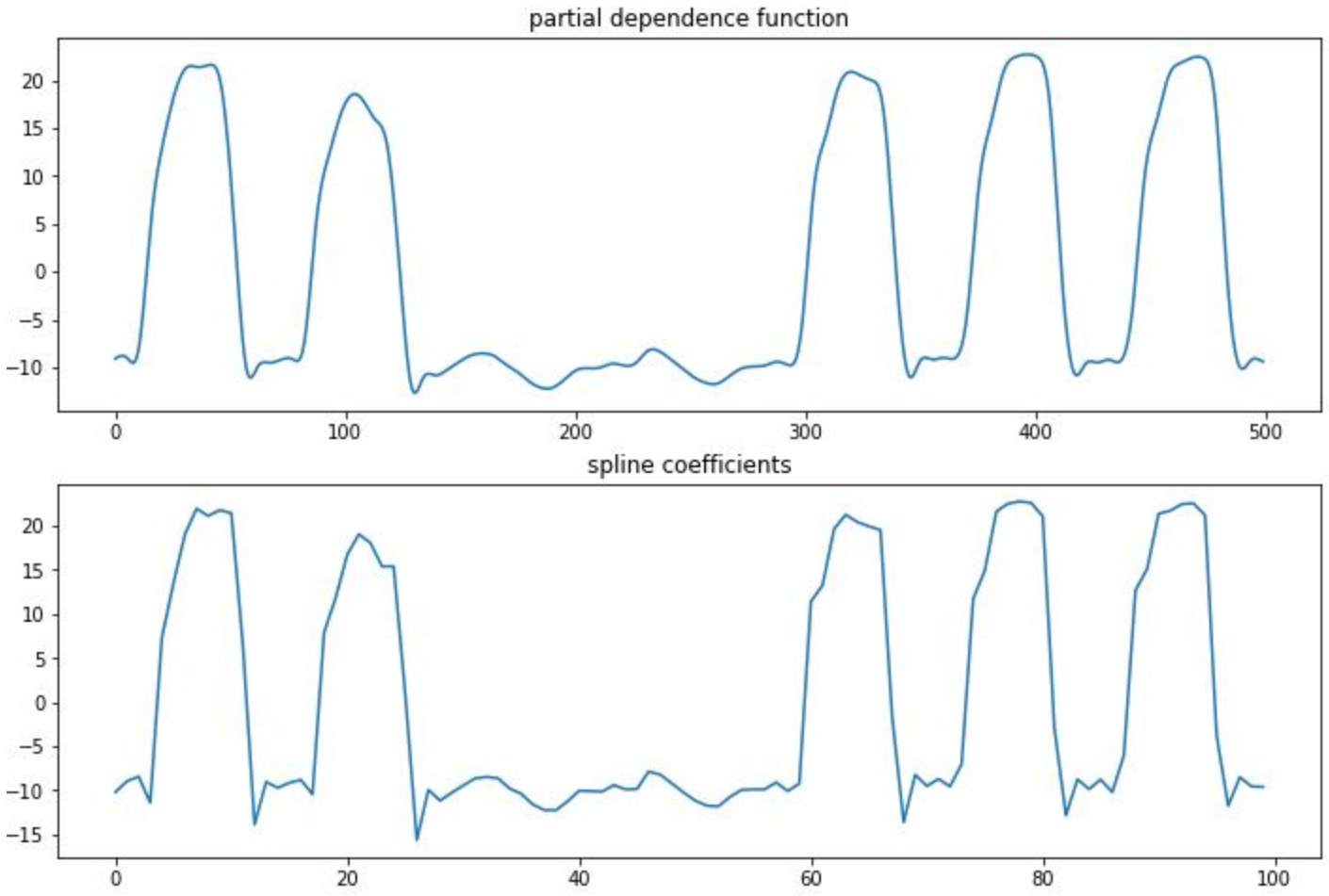
$$||y - X\beta||^2 + \lambda \int_a^b [f''(x)]^2 dx$$

Smoothing

2 modifications:

- Compute on spline coefficients β
- Use numerical derivatives + integrals

Smoothing


partial dependence function
20
15
10
5
0
−5
−10
0
100
200
300
400
500
spline coefficients
20
15
10
5
0
−5
−10
−15
0
20
40
60
80
100

Smoothing

numerical derivatives

minimize

$$||y - X\beta||^2 + \lambda\beta^\top S\beta$$

model coefficients

Smoothing

minimize

$$\beta = (X^\top X + \lambda S)^{-1} X^\top y$$

Smoothing

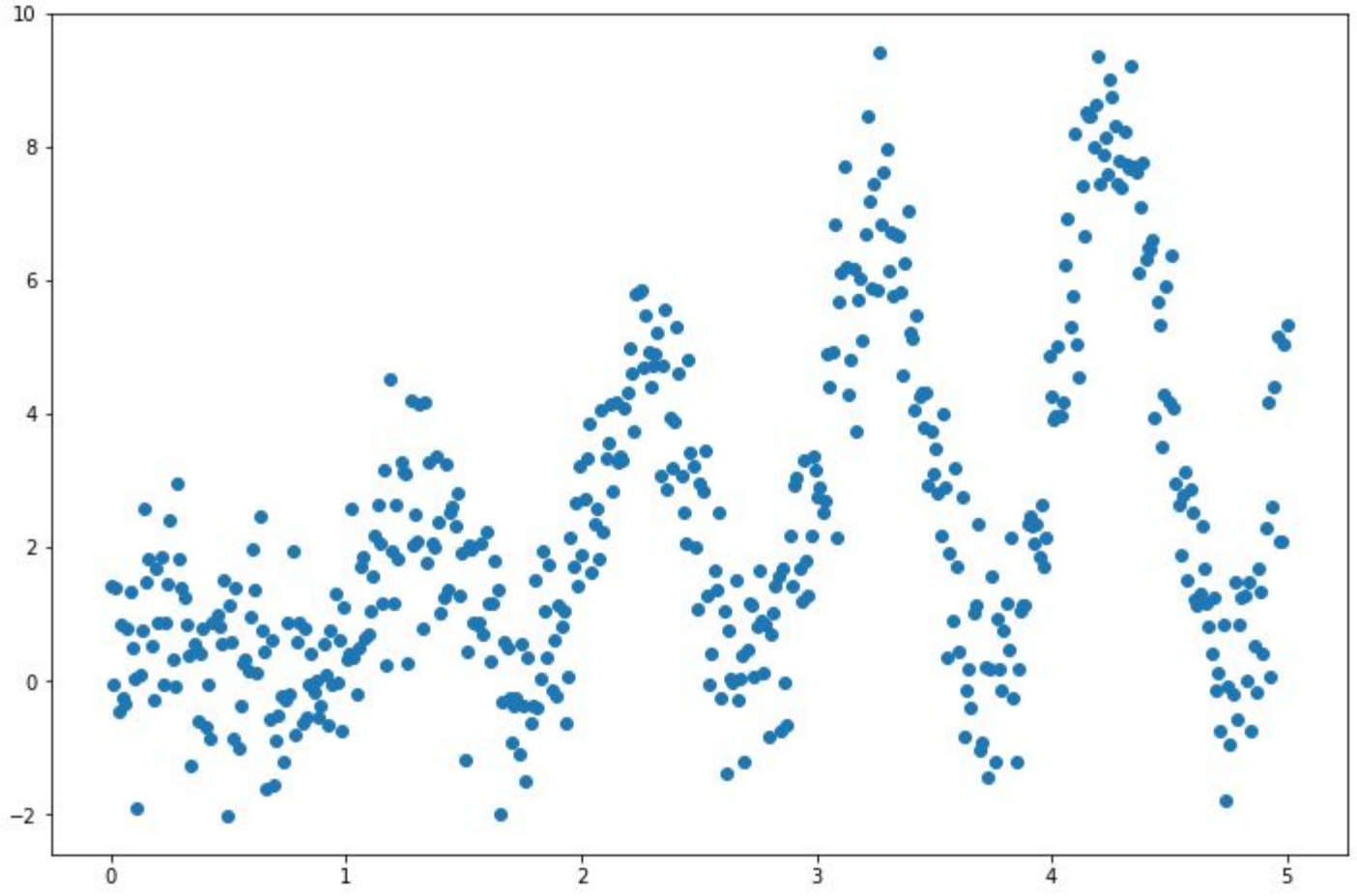
Similar to ridge regression

$$\beta = (X^\top X + \lambda I)^{-1} X^\top y$$

Smoothing

```
X = np.linspace(0, 5, 500)
y = np.sin(X * 2 * np.pi)*X + X + np.random.randn(len(X))

plt.scatter(X, y)
```

Smoothing



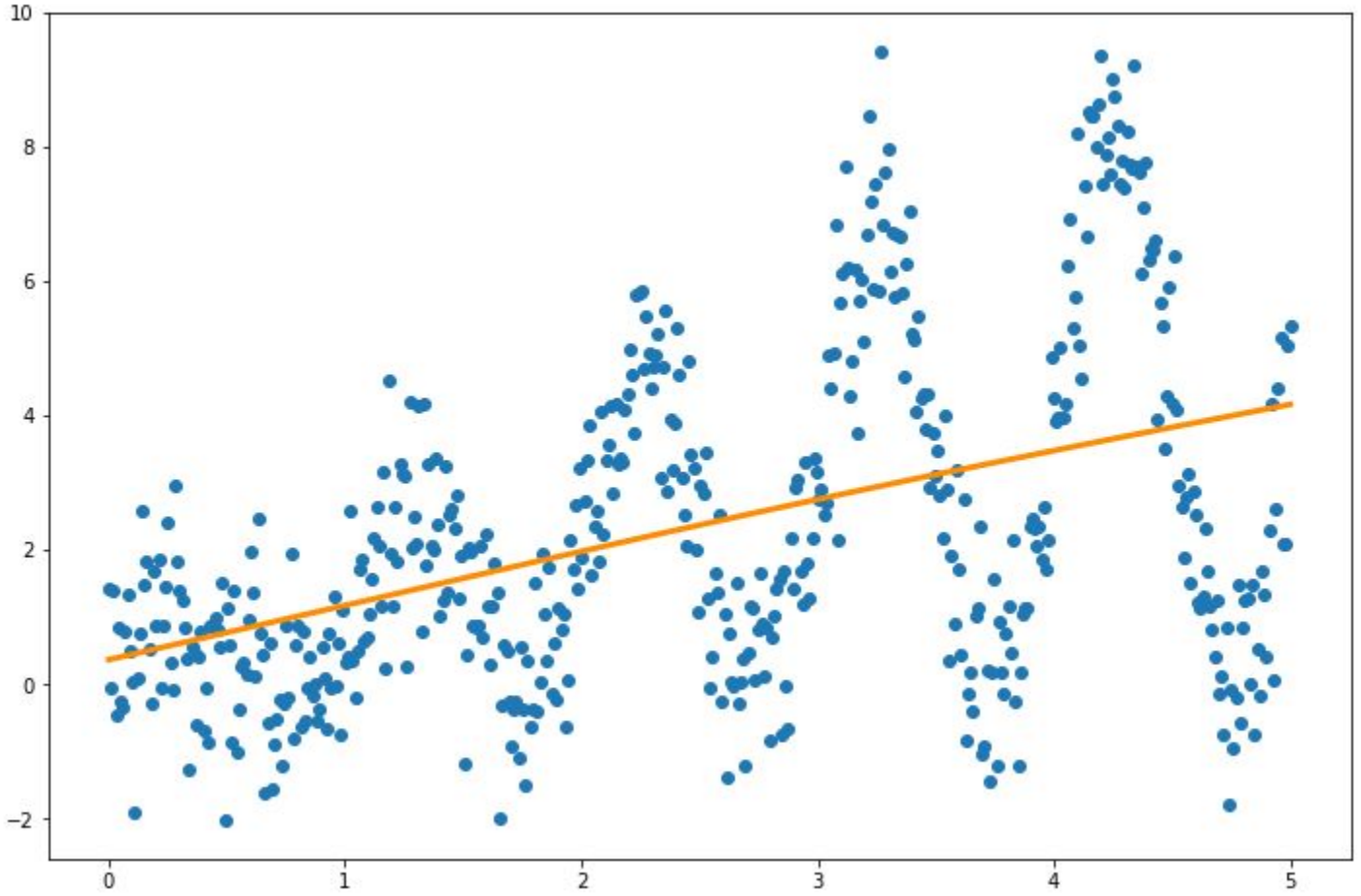
Smoothing

```
from pygam import LinearGAM

# high lambda forces a straight line
gam = LinearGAM(lam=1e6, n_splines=50).fit(X, y)
```

Smoothing

```
from pygam import LinearGAM

# high lambda forces a straight line
gam = LinearGAM(lam=1e6, n_splines=50).fit(X, y)
```

Smoothing




```
# generate a nice grid
XX = gam.generate_X_grid()
plt.plot(XX, gam.predict(XX))
```

Smoothing

```
>> gam.summary()
```

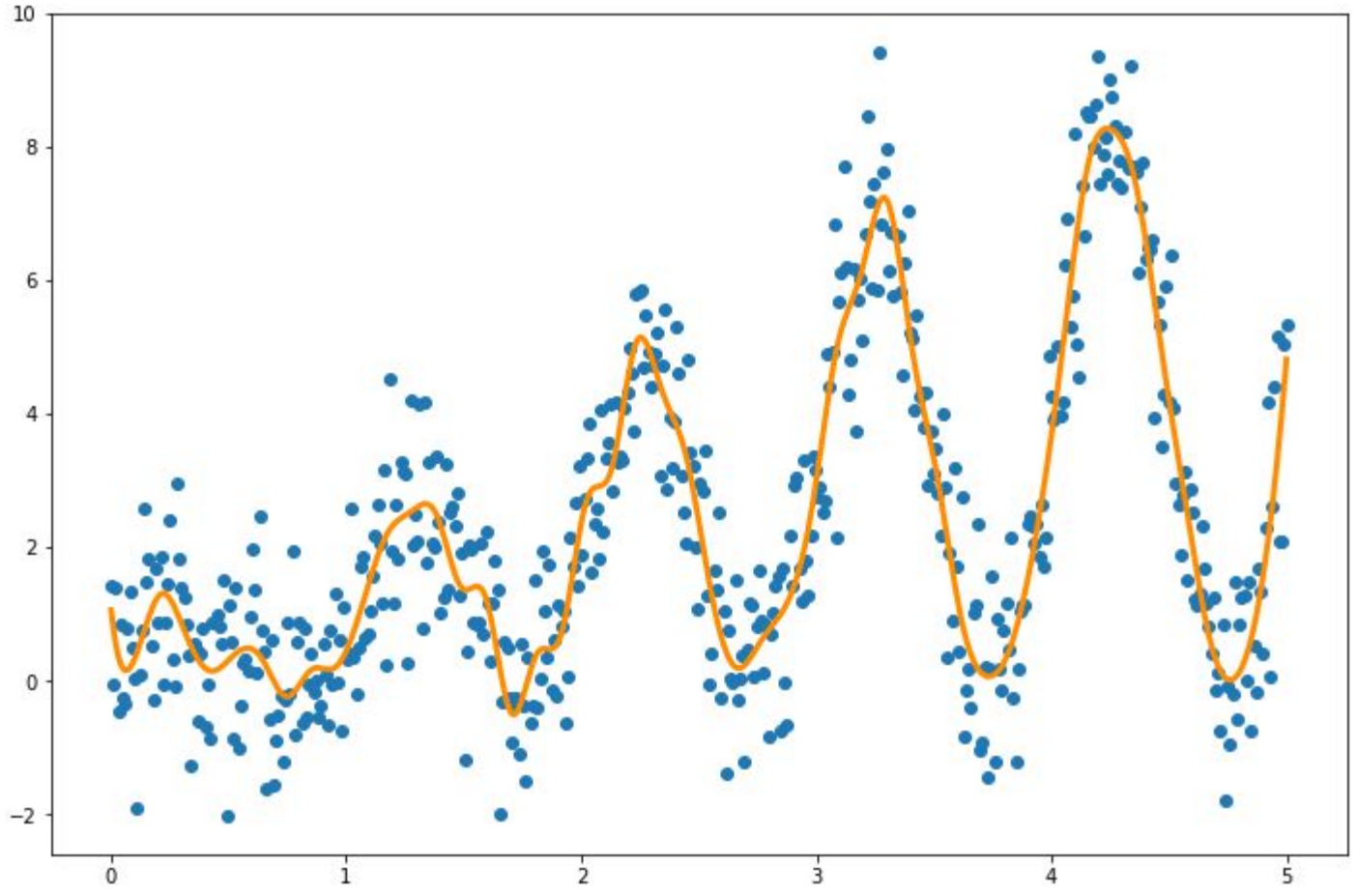
Smoothing

```
LinearGAM
============================================= ==========================================================
Distribution:                      NormalDist Effective DoF:                                     1.1141
Link Function:                    IdentityLink Log Likelihood:                                -1339.885
Number of Samples:                         500 AIC:                                           2685.9981
                                               AICc:                                          2686.0498
                                               GCV:                                              5.3358
                                               Scale:                                            5.2952
                                               Pseudo R-Squared:                                 0.2076
=================================================================================================================
Feature Function    Data Type      Num Splines   Spline Order  Linear Fit  Lambda     P > x      Sig. Code
================== ============= ============ ============ =========== ========== ========== ==========
feature 1          numerical      50            3             False       1000000.0  1.11e-16   ***
intercept                                                                           1.11e-16   ***
=================================================================================================================
Significance codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

WARNING: Fitting splines and a linear function to a feature introduces a model identifiability problem
         which can cause p-values to appear significant when they are not.

WARNING: p-values calculated in this manner behave correctly for un-penalized models or models with
         known smoothing parameters, but when smoothing parameters have been estimated, the p-values
         are typically lower than they should be, meaning that the tests reject the null too readily.
```

Smoothing

```
# tiny lambda is super flexible
gam = LinearGAM(lam=1e-6, n_splines=50).fit(X, y)
```

Smoothing



Smoothing

```
LinearGAM
============================================= ==========================================================
Distribution:                      NormalDist Effective DoF:                                     48.9993
Link Function:                    IdentityLink Log Likelihood:                                  -674.2603
Number of Samples:                        500 AIC:                                             1450.5194
                                              AICc:                                            1462.3583
                                              GCV:                                                1.1718
                                              Scale:                                               0.963
                                              Pseudo R-Squared:                                   0.8616
==========================================================================================================
Feature Function   Data Type      Num Splines   Spline Order  Linear Fit  Lambda     P > x      Sig. Code
================== ============== ============ ============ =========== ========== ========== ==========
feature 1          numerical      50            3             False       0.0        1.11e-16   ***
intercept                                                                          1.11e-16   ***
==========================================================================================================
Significance codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

WARNING: Fitting splines and a linear function to a feature introduces a model identifiability problem
         which can cause p-values to appear significant when they are not.

WARNING: p-values calculated in this manner behave correctly for un-penalized models or models with
         known smoothing parameters, but when smoothing parameters have been estimated, the p-values
         are typically lower than they should be, meaning that the tests reject the null too readily.
```

Smoothing

So how do we choose the **right** amount of smoothing?

- Cross validation!

Smoothing

pyGAM computes GCV

- Fast approximation to Leave-One-Out CV

$$\frac{n||\boldsymbol{y}-\hat{\boldsymbol{\mu}}||}{(n-tr(A))^2}$$

Smoothing

pyGAM computes GCV

- Fast approximation to Leave-One-Out CV

$$\frac{n||\boldsymbol{y}-\hat{\boldsymbol{\mu}}||}{(n-edof)^2}$$

Smoothing

```
gam = LinearGAM(n_splines=50).fit(X, y)
```

Smoothing

```
gam = LinearGAM(n_splines=50).gridsearch(X, y)
```

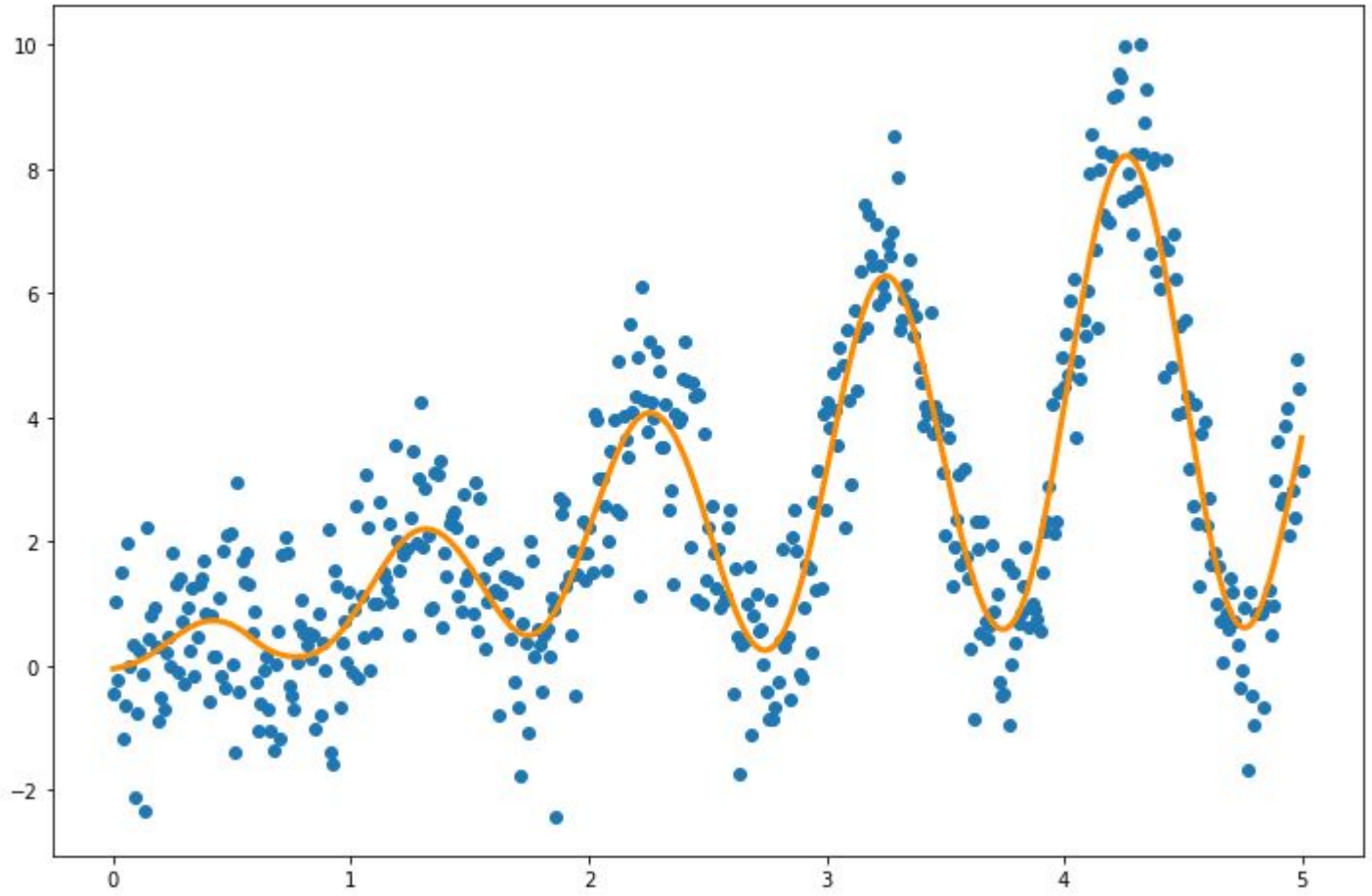
Smoothing

```
lams = np.logspace(-4, 0, 100)
gam = LinearGAM(n_splines=50).gridsearch(X, y, lam=lams)
```

Smoothing

```
LinearGAM
============================================= ==========================================================
Distribution:                      NormalDist Effective DoF:                                     25.1906
Link Function:                    IdentityLink Log Likelihood:                                  -692.0659
Number of Samples:                        500 AIC:                                             1438.5129
                                              AICc:                                            1441.7621
                                              GCV:                                                1.0855
                                              Scale:                                              0.9836
                                              Pseudo R-Squared:                                   0.8477
==========================================================================================================
Feature Function   Data Type      Num Splines   Spline Order  Linear Fit  Lambda     P > x      Sig. Code
================== ============== ============ ============ =========== ========== ========== ==========
feature 1          numerical      50            3             False       1.0        1.11e-16   ***
intercept                                                                          1.11e-16   ***
==========================================================================================================
Significance codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

WARNING: Fitting splines and a linear function to a feature introduces a model identifiability problem
         which can cause p-values to appear significant when they are not.

WARNING: p-values calculated in this manner behave correctly for un-penalized models or models with
         known smoothing parameters, but when smoothing parameters have been estimated, the p-values
         are typically lower than they should be, meaning that the tests reject the null too readily.
```

Smoothing



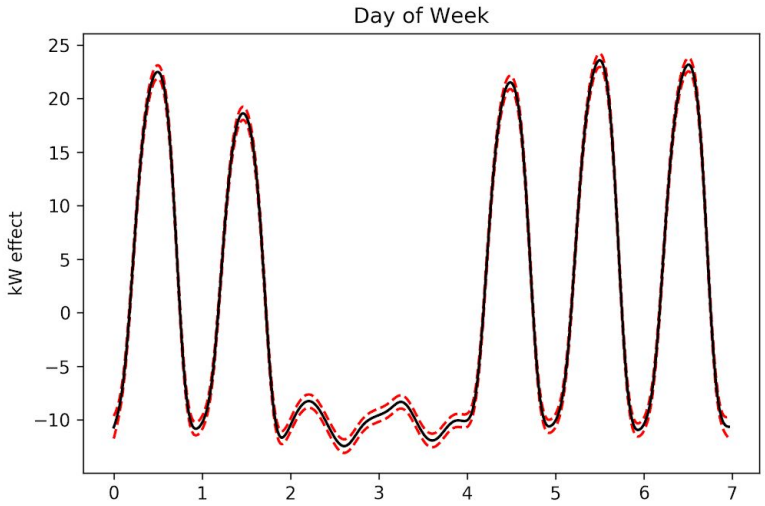
Back at PyDatatopolis

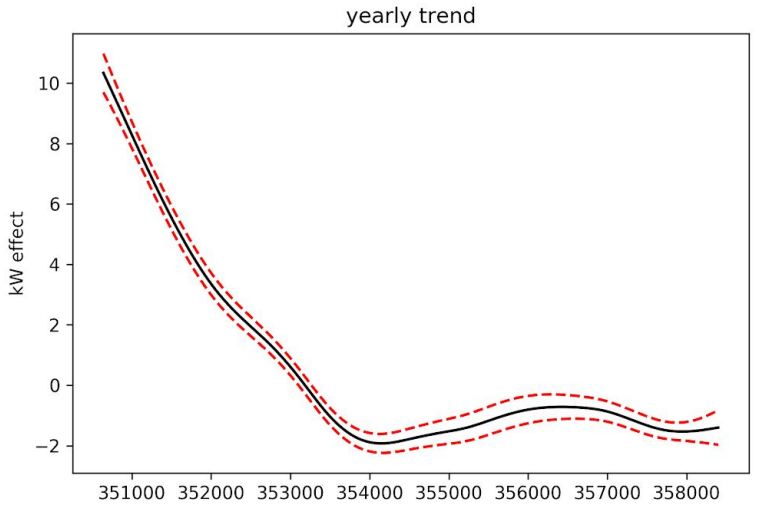
- Select right amount of smoothing
- Cloud cover?

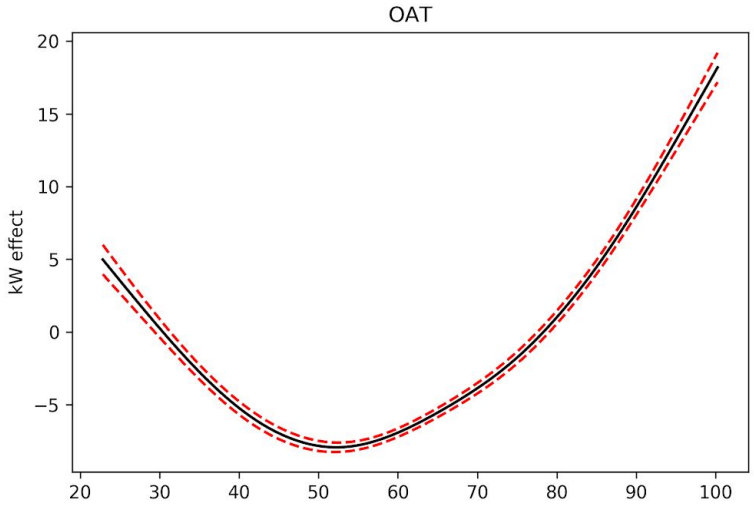
Back at PyDatatopolis

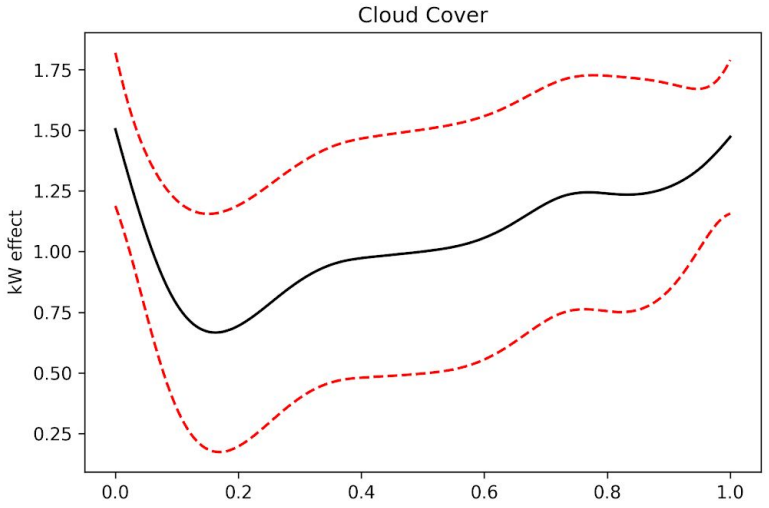
```
dist = np.random.uniform(1e-3, 1e3, (100,4))

gam = LinearGAM(n_splines=[100,25,25,25]).gridsearch(X, y, lam=dist)
```

Back at PyDatatopolis









Back at PyDatatopolis

```
LinearGAM
============================================= ==========================================================
Distribution:                        NormalDist Effective DoF:                                     56.6547
Link Function:                     IdentityLink Log Likelihood:                                -32515.6534
Number of Samples:                         7759 AIC:                                            65146.6162
                                                AICc:                                           65147.4945
                                                GCV:                                               26.2008
                                                Scale:                                             25.8566
                                                Pseudo R-Squared:                                   0.8865
=================================================================================================================
Feature Function   Data Type      Num Splines   Spline Order  Linear Fit  Lambda     P > x      Sig. Code
================== ============== ============= ============= =========== ========== ========== ==========
feature 1          numerical      100           3             False       36.4721    1.11e-16   ***
feature 2          numerical      25            3             False       229.9264   1.11e-16   ***
feature 3          numerical      25            3             False       938.4219   1.11e-16   ***
feature 4          numerical      25            3             False       430.7849   4.70e-01
intercept                                                                           1.11e-16   ***
=================================================================================================================
Significance codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Future work

Lots of cool features…

- Feature interactions
- Periodicity constraints
- Direct smoothing parameter optimization
- ExpectileGAM
- …

https://github.com/dswah/pyGAM/issues

Vielen Dank!

Questions?

- Can pyGAM do classification?
- What other distributions can we model?
- What size of data can pyGAM handle?
- Patsy compatible?

Some math...