Session 12:

Supervised learning, part 1

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Agenda

1. Modelling data
2. A familiar regression model
3. The curse of overfitting
4. Important details

Vaaaamos

In [18]:

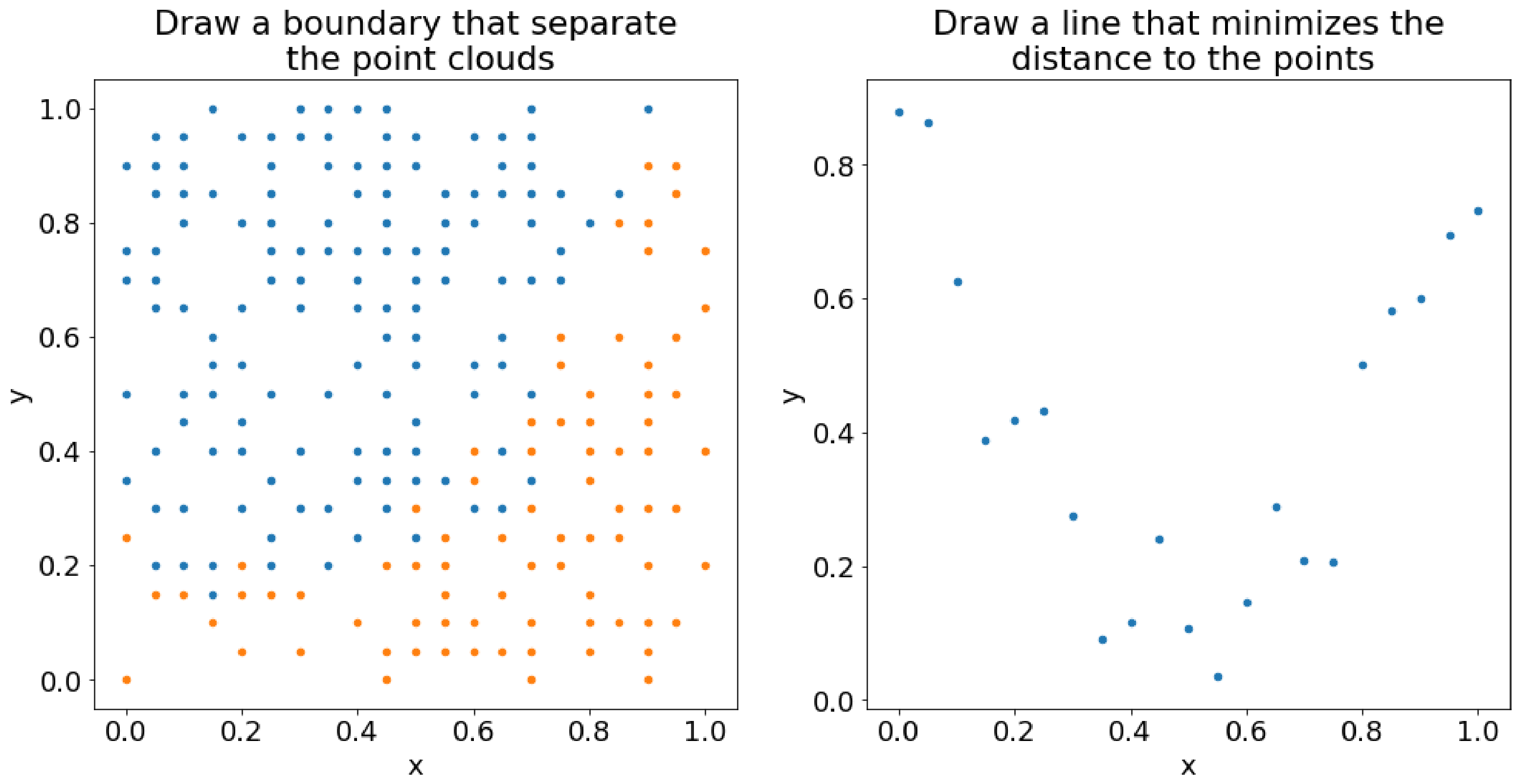
```
import warnings
from sklearn.exceptions import ConvergenceWarning
warnings.filterwarnings(action='ignore', category=ConvergenceWarning)

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns

plt.style.use('default') # set style (colors, background, size, gridlines etc.)
plt.rcParams['figure.figsize'] = 10, 4 # set default size of plots
plt.rcParams.update({'font.size': 18})
```

Supervised problems (1)

How do we distinguish between problems?

In [19]:
```
f_identify_question
```

Out[19]:

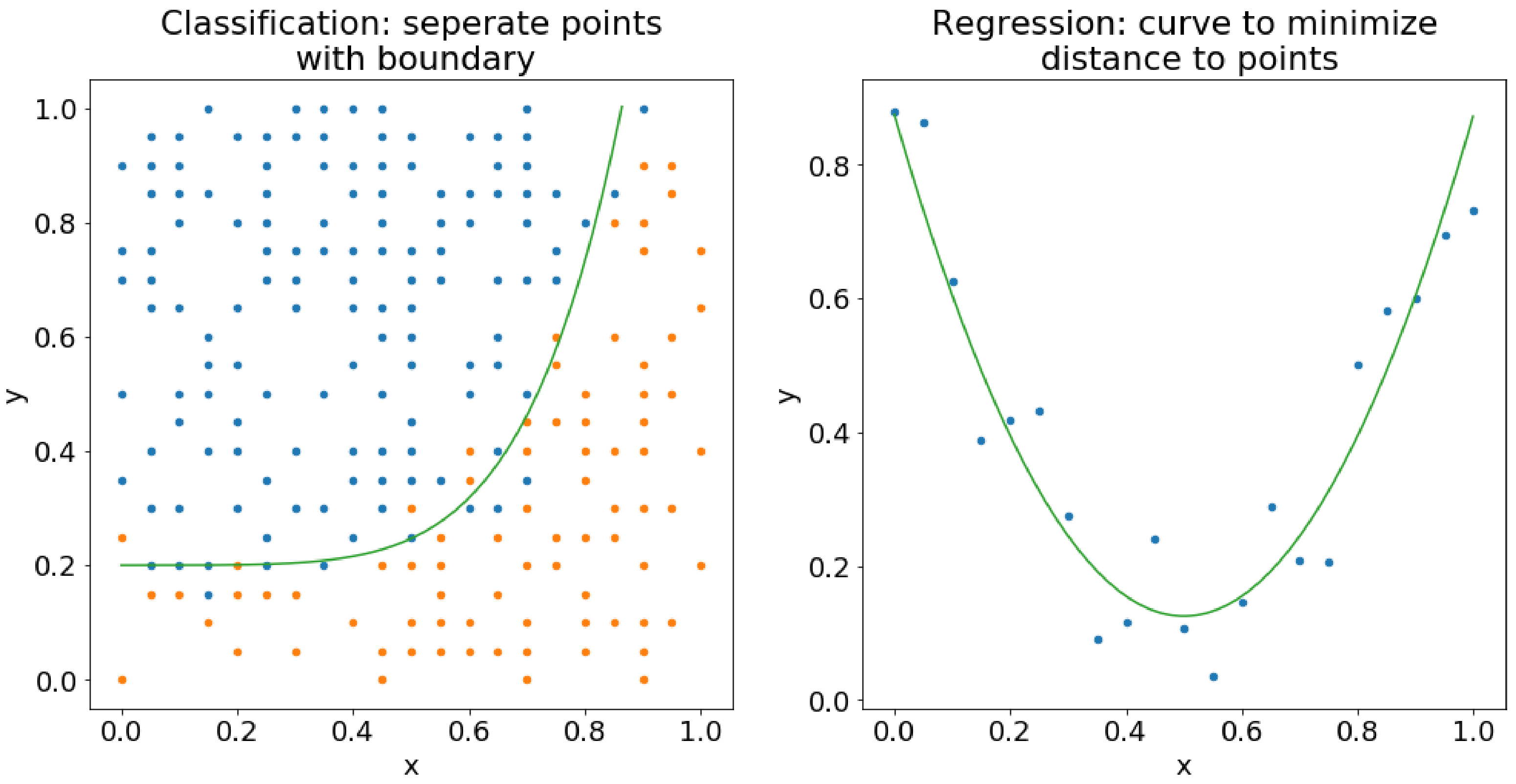


Supervised problems (2)

The two canonical problems

In [20]:
```
f_identify_answer
```

Out[20]:



Supervised problems (3)

Which models have we seen for classification?

- .
- .
- .

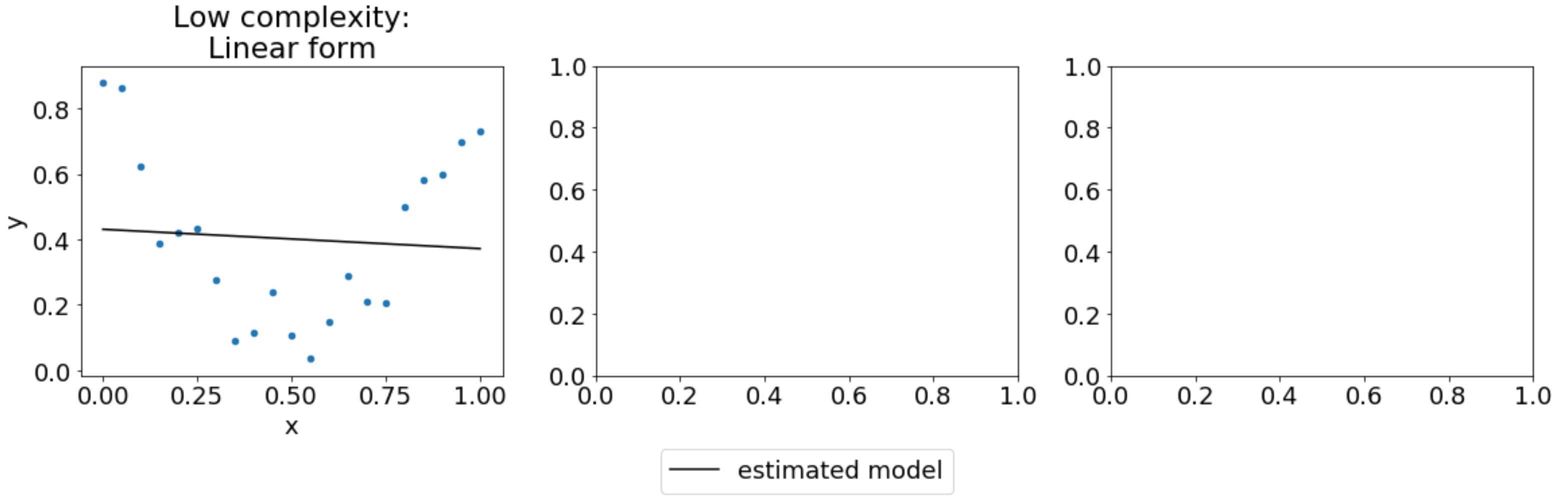
Modelling data

Model complexity (1)

What does a model of low complexity look like?

In [21]:
```
f_complexity[0]
```

Out[21]:

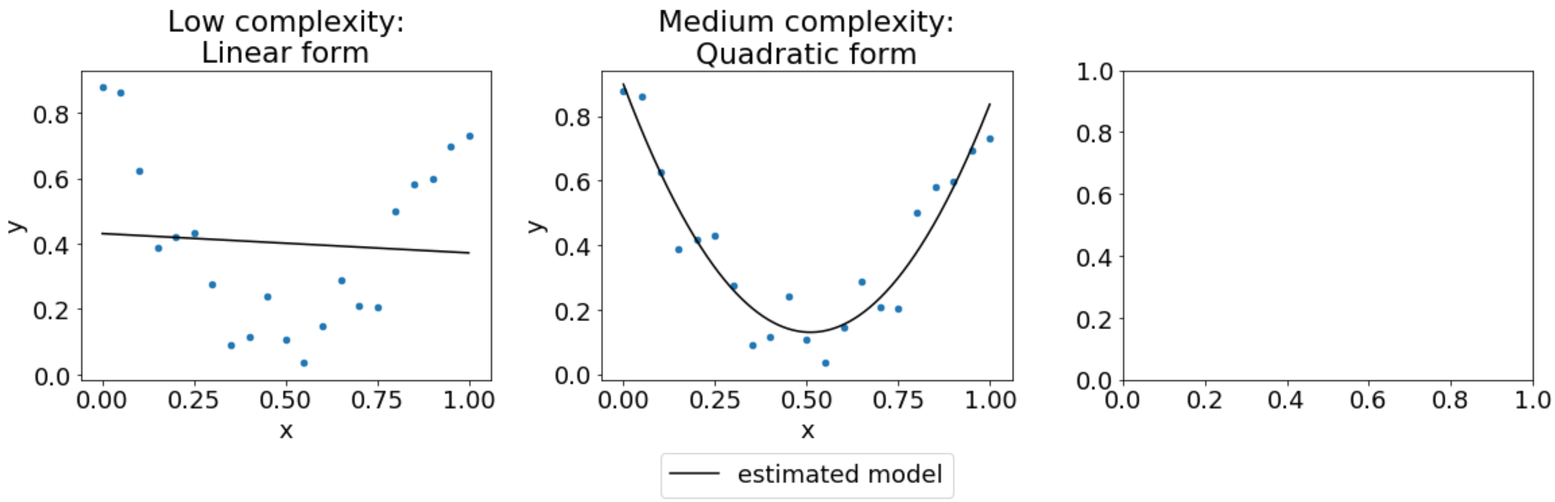


Model complexity (2)

What does medium model complexity look like?

In [22]:
```
f_complexity[1]
```

Out[22]:

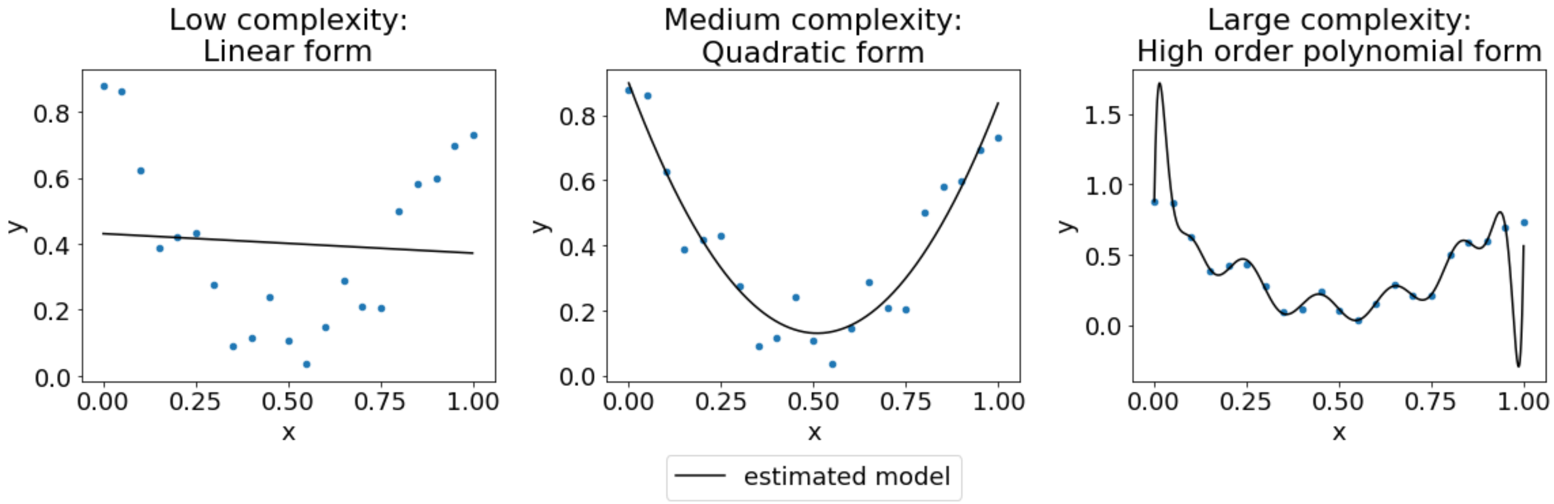


Model complexity (3)

What does high model complexity look like?

In [23]:
```
f_complexity[2]
```

Out[23]:



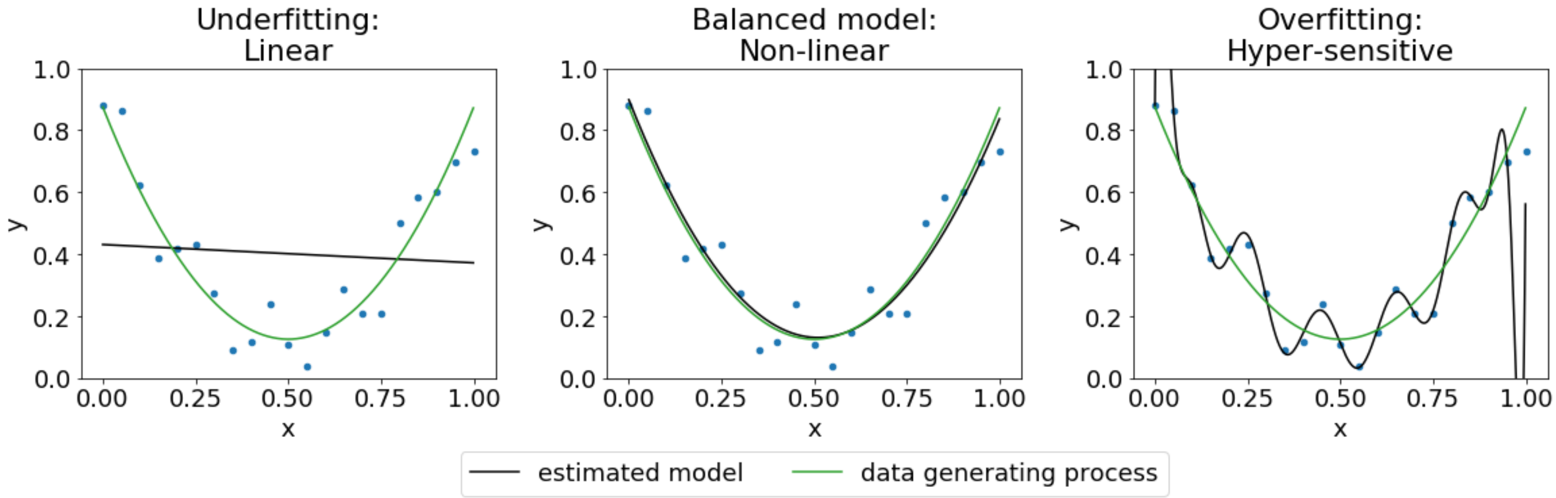
Model fitting (1)

Quiz (1 min.): Which model fitted the data best?

In [24]:

```
f_bias_var['regression'][2]
```

Out[24]:

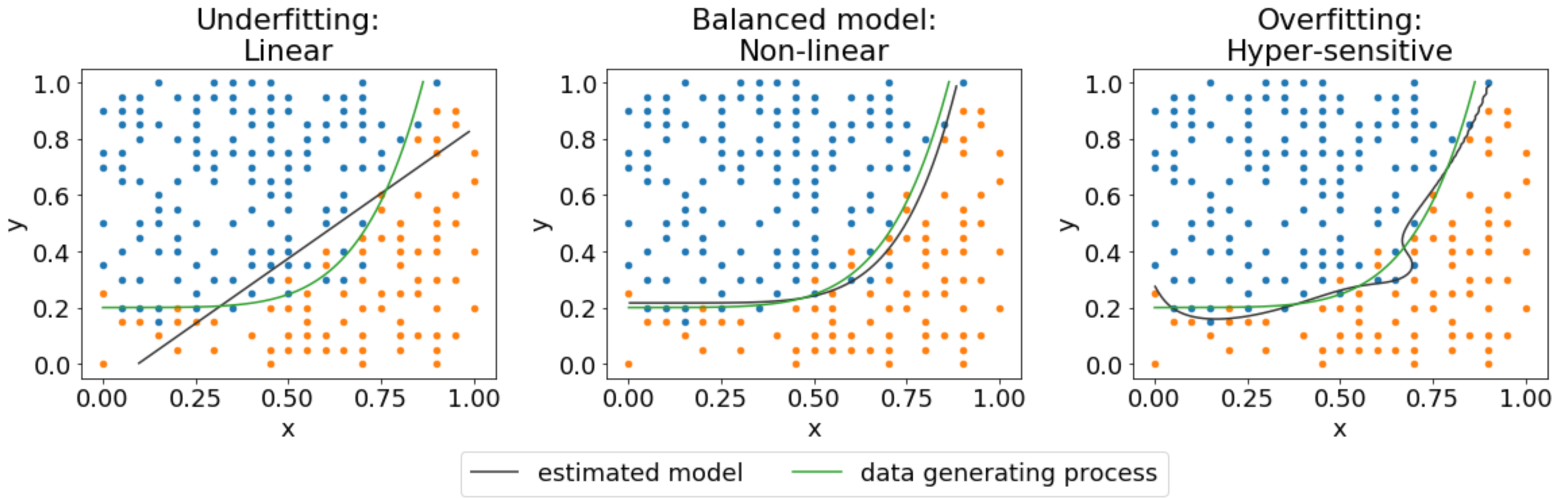


Model fitting (2)

What does underfitting and overfitting look like for classification?

In [25]:
```
f_bias_var['classification'][2]
```

Out[25]:



Two agendas (1)

What are the objectives of empirical research?

1. *causation*: what is the effect of a particular variable on an outcome?
2. *prediction*: find some function that provides a good prediction of y as a function of x

Two agendas (2)

How might we express the agendas in a model?

$$y = \alpha + \beta x + \varepsilon$$

- *causation*: interested in $\hat{\beta}$
- *prediction*: interested in $\hat{y}$

Two agendas (3)

Might these two agendas be related at a deeper level? Can prediction quality inform us about how to make causal models?

A familiar regression model

Estimation (1)

Do we know already some ways to estimate regression models?

- Social scientists know all about the Ordinary Least Squares (OLS).
  - OLS estimate both parameters and their standard deviation.
  - Is best linear unbiased estimator under regularity conditions.

How is OLS estimated?

- $\beta = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- computation requires non perfect multicollinarity.

Estimation (2)

How might we estimate a linear regression model?

- first order method (e.g. gradient descent)
- second order method (e.g. Newton-Raphson)

So what the hell was gradient descent?

- compute errors, multiply with features and update

Estimation (3)

Can you explain that in details?

- Yes, like with Adaline, we minimize the sum of squared errors (SSE):

$$SSE = \boldsymbol{e}^T\boldsymbol{e}$$

$$\boldsymbol{e} = \mathbf{y} - \mathbf{X}\mathbf{w}$$

In [26]:

```
X = np.random.normal(size=(3,2))
y = np.random.normal(size=(3))
w = np.random.normal(size=(3))

e = y-(w[0]+X.dot(w[1:]))
SSE = e.T.dot(e)
```

Estimation (4)

And what about the updating..? What is it something about the first order deritative?

$$\frac{\partial SSE}{\partial \hat{w}} = \mathbf{X}^T \mathbf{e},$$
$$\Delta \hat{w} = \eta \cdot \mathbf{X}^T \mathbf{e} = \eta \cdot \mathbf{X}^T (\mathbf{y} - \hat{\mathbf{y}})$$

In [27]:

```
eta = 0.001 # learning rate
fod = X.T.dot(e)
update_vars = eta*fod
update_bias = eta*e.sum()
```

Estimation (5)

What might some advantages be relative to OLS?

- Works despite high multicollinearity
- Speed
  - OLS has $\mathcal{O}(K^2N)$ computation time (read more (https://math.stackexchange.com/questions/84495/computational-complexity-of-least-square-regression-operation))
    - Quadratic scaling in number of variables (K).
  - Stochastic gradient descent
    - Likely to converge faster with many observations (N)

Fitting a polynomial (1)

Polyonomial: $f(x) = 2 + 8 * x^4$

Try models of increasing order polynomials.

- Split data into train and test (50/50)
- For polynomial order 0 to 9:
  - Iteration n: $y = \sum_{k=0}^{n} (\beta_k \cdot x^k) + \varepsilon.$
  - Estimate order n model on training data
  - Evaluate with on test data with RMSE:
    - $logRMSE = \log(\sqrt{MSE})$

Fitting a polynomial (2)

We generate samples of data from true model.

In [28]:

```
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression

def true_fct(X):
    return 2+X**4

n_samples = 25
n_degrees = 15

np.random.seed(0)

X_train = np.random.normal(size=(n_samples,1))
y_train = true_fct(X_train).reshape(-1) + np.random.randn(n_samples)

X_test = np.random.normal(size=(n_samples,1))
y_test = true_fct(X_test).reshape(-1) + np.random.randn(n_samples)
```

Fitting a polynomial (3)

We estimate the polynomials

In [29]:

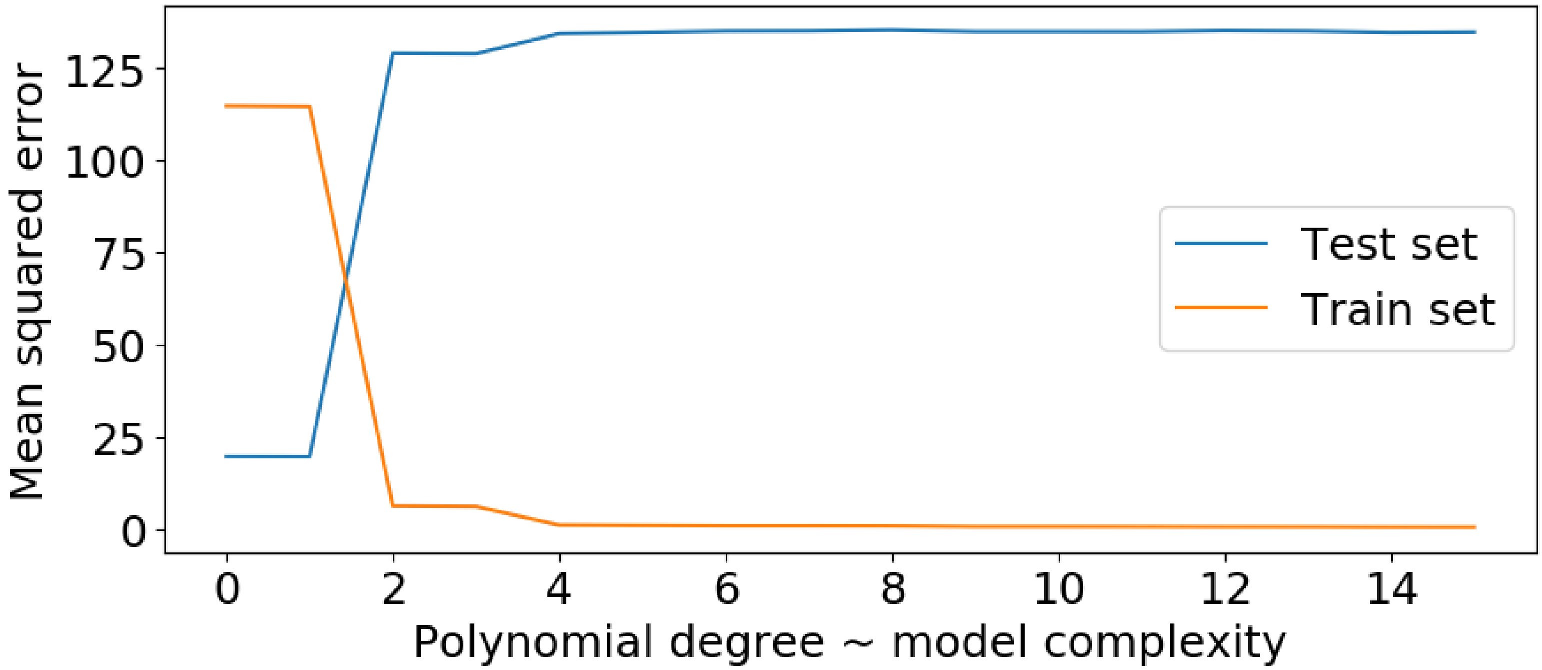
```
from sklearn.metrics import mean_squared_error as mse

test_mse = []
train_mse = []
parameters = []
degrees = range(n_degrees+1)

for p in degrees:
    X_train_p = PolynomialFeatures(degree=p).fit_transform(X_train)
    X_test_p = PolynomialFeatures(degree=p).fit_transform(X_train)
    reg = LinearRegression().fit(X_train_p, y_train)
    train_mse += [mse(reg.predict(X_train_p),y_train)]
    test_mse += [mse(reg.predict(X_test_p),y_test)]
    parameters.append(reg.coef_)
```

Fitting a polynomial (4)

So what happens to the model performance in- and out-of-sample?

In [30]:
```
degree_index = pd.Index(degrees,name='Polynomial degree ~ model complexity')
ax = pd.DataFrame({'Train set':train_mse, 'Test set':test_mse})\
    .set_index(degree_index)\
    .plot(figsize=(10,4))
ax.set_ylabel('Mean squared error')
```

Out[30]:
```
Text(0,0.5,'Mean squared error')
```



Fitting a polynomial (4)

Why does it go wrong?

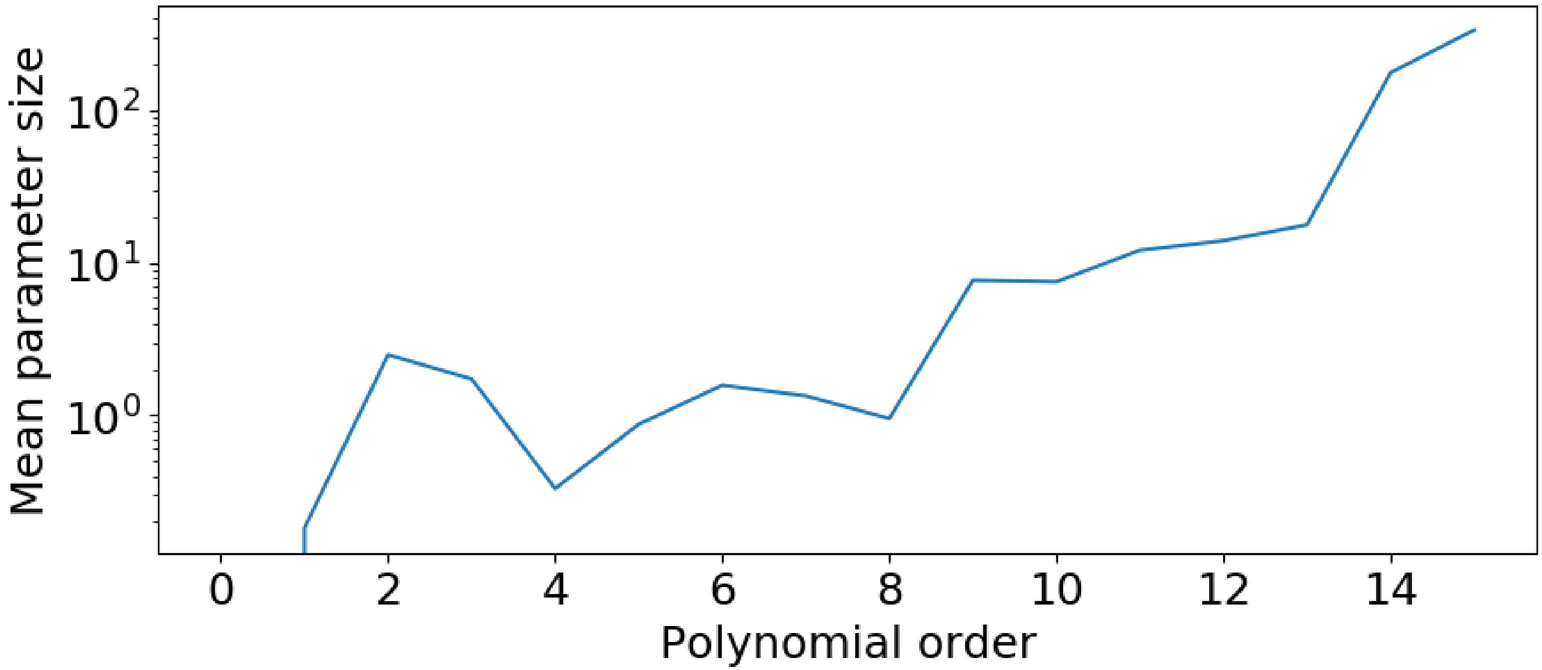
- more spurious parameters
- the coefficient size increases

Fitting a polynomial (5)

What do you mean coefficient size increase?

In [31]:
```
order_idx = pd.Index(range(n_degrees+1),name='Polynomial order')
ax = pd.DataFrame(parameters,index=order_idx)\
.abs().mean(1)\
.plot(logy=True)
ax.set_ylabel('Mean parameter size')
```

Out[31]:
```
Text(0,0.5,'Mean parameter size')
```

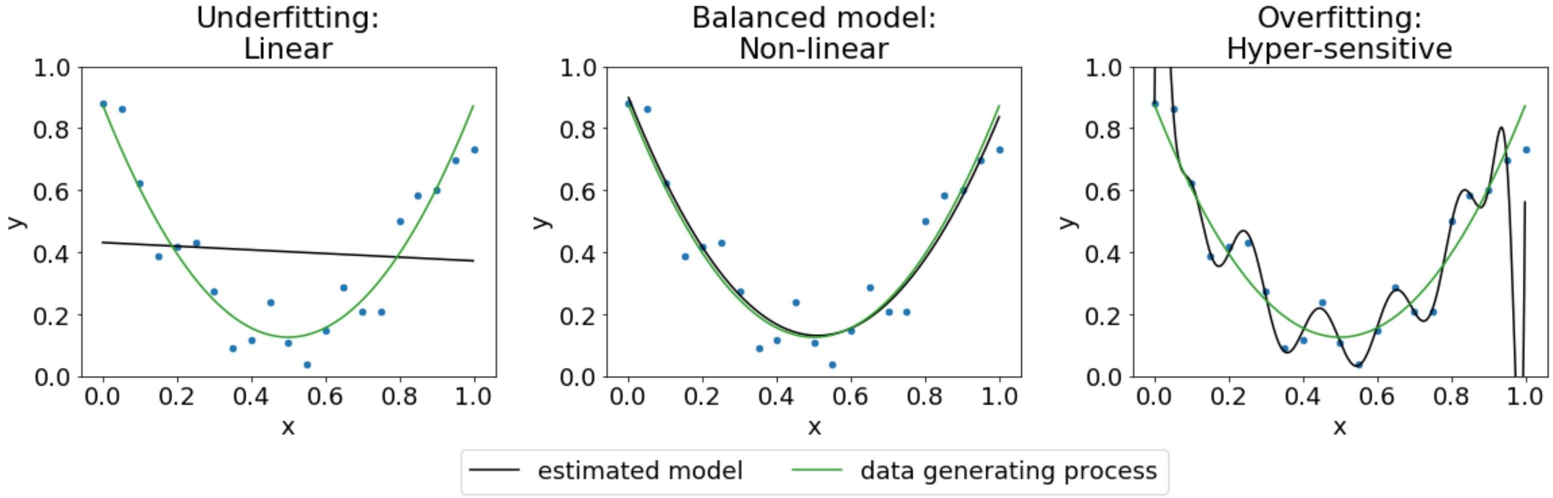


Fitting a polynomial (6)

How else could we visualize this problem?

In [16]:
```
f_bias_var['regression'][2]
```

Out[16]:



The curse of overfitting

Looking for a remedy

How might we solve the overfitting problem?

- .
- .

Regularization (1)

Why do we regularize?

- To mitigate overfitting > better model predictions

How do we regularize?

- We make models which are less complex:
    - reducing the **number** of coefficient;
    - reducing the **size** of the coefficients.

Regularization (2)

What does regularization look like?

We add a penalty term our optimization procedure:

$$\arg\min_\beta \underbrace{E[(y_0 - \hat{f}(x_0))^2]}_{\text{MSE}} + \underbrace{\lambda \cdot R(\beta)}_{\text{penalty}}$$

Introduction of penalties implies that increased model complexity has to be met with high increases precision of estimates.

Regularization (3)

What are some used penalty functions?

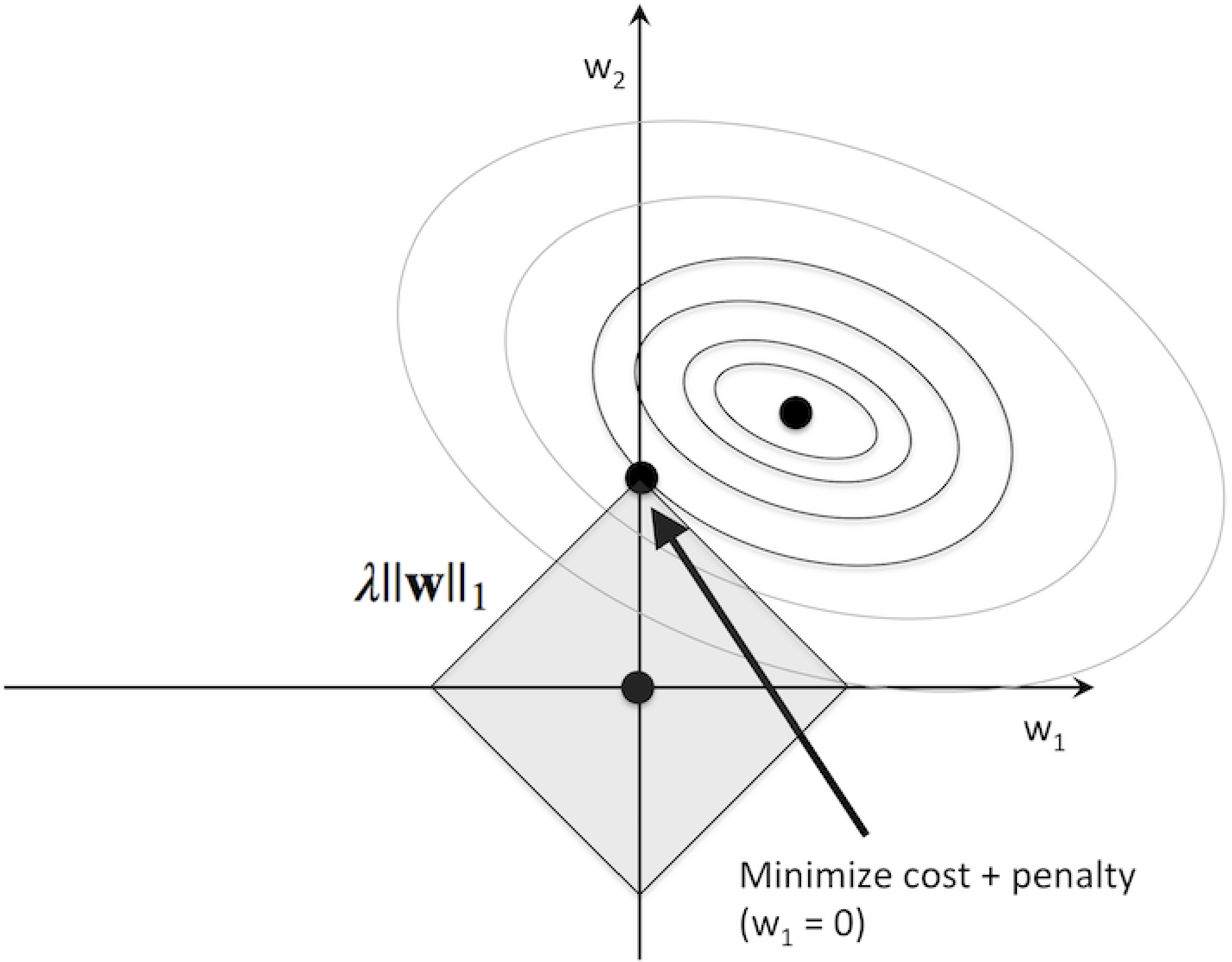
The two most common penalty functions are L1 and L2 regularization.

- L1 regularization (***Lasso***): $R(\beta) = \sum_{j=1}^{p} |\beta_j|$
  - Makes coefficients sparse, i.e. selects variables by removing some (if λ is high)
- L2 regularization (***Ridge***): $R(\beta) = \sum_{j=1}^{p} \beta_j^2$
  - Reduce coefficient size
  - Fast due to analytical solution

To note: The *Elastic Net* uses a combination of L1 and L2 regularization.

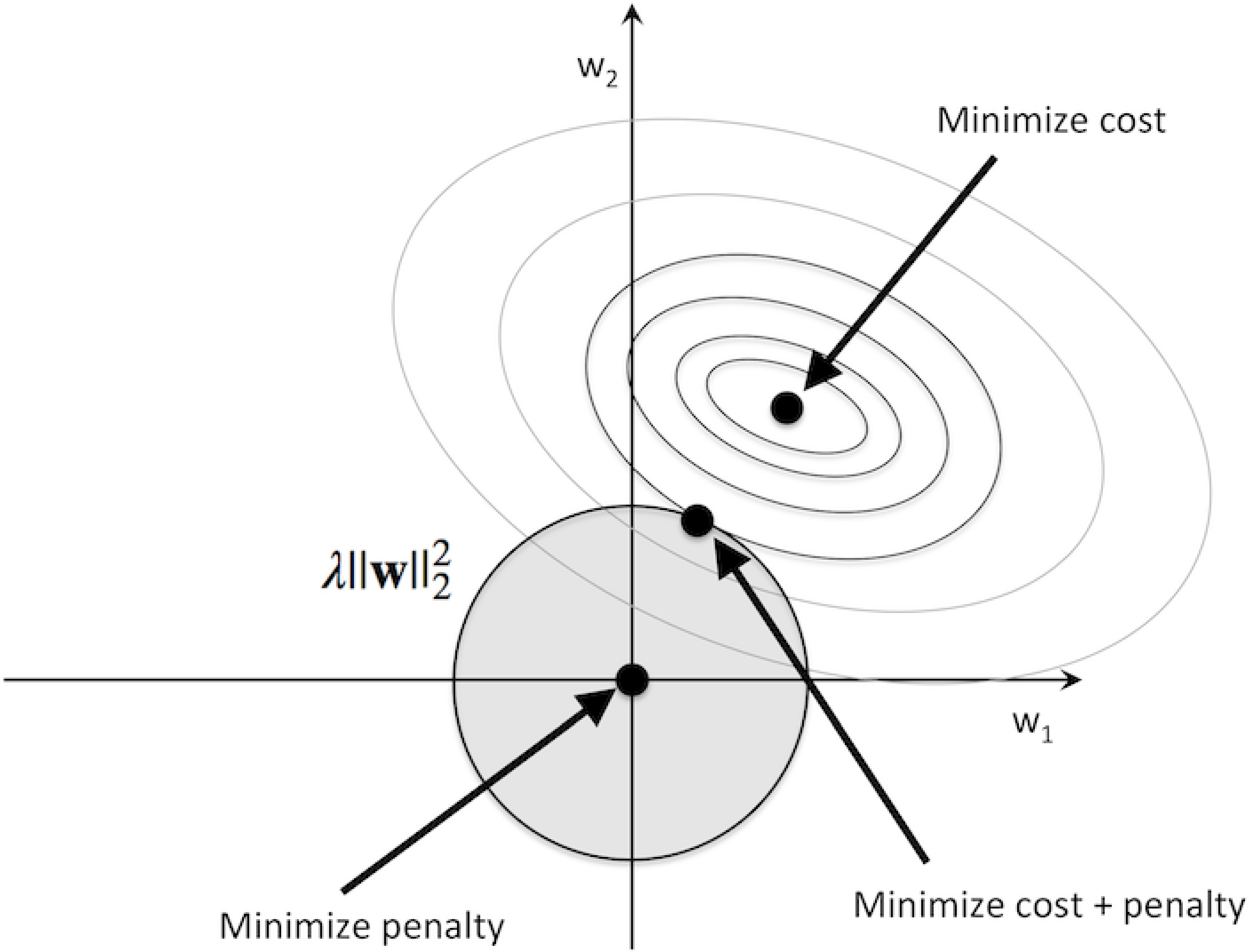
Regularization (4)

How the Lasso (L1 reg.) deviates from OLS



Regularization (5)

How the Ridge regression (L2 reg.) deviates from OLS



Regularization (6)

How might we describe the λ of Lasso and Ridge?

These are hyperparameters that we can optimize over.

- More about this tomorrow.

Implementation details

The devils in the details (1)

So we just run regularization?

NO

We need to rescale our features:

- convert to zero mean:
- standardize to unit std:

Compute in Python:

- option 1: `StandardScaler` in `sklearn`
- option 2: `(X - np.mean(X)) / np.std(X)`

The devils in the details (2)

So we just scale our test and train?

NO

Fit to the distribution in the training data first, then rescale train and test! See more here (https://stats.stackexchange.com/questions/174823/how-to-apply-standardization-normalization-to-train-and-testset-if-prediction-i).

The devils in the details (3)

So we just rescale before using polynomial features?

NO

Otherwise the interacted varaibles are not gaussian distributed.

The devils in the details (4)

Does sklearn's `PolynomialFeatures` work for more than variable?

YES!

The end

Return to agenda