Introduction to Machine Learning
Nonlinear Regression

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August 6, 2019

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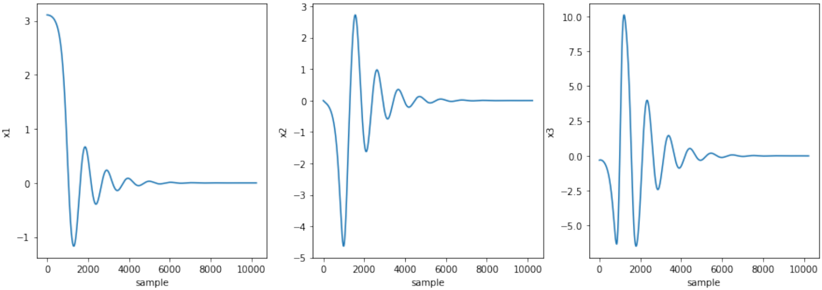
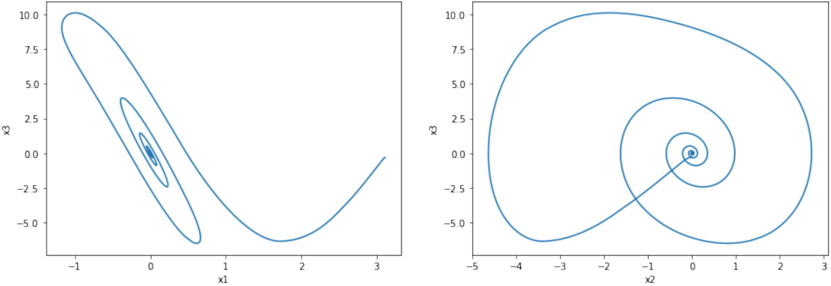
System identification with linear regression

Can we find the length of a pendulum given measured data from it?



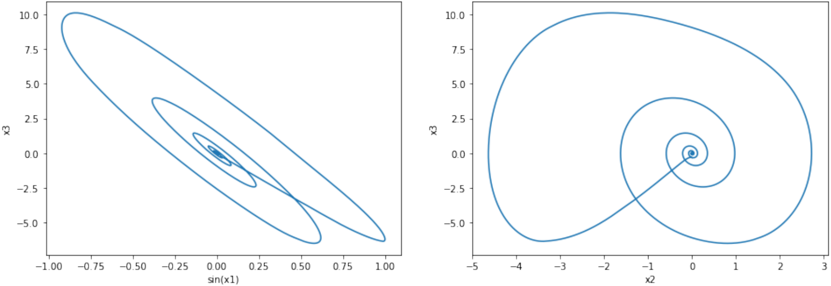
System identification with linear regression

The relationship between x_1 and x_3 is nonlinear



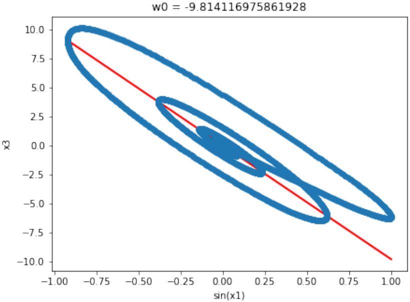
System identification with linear regression

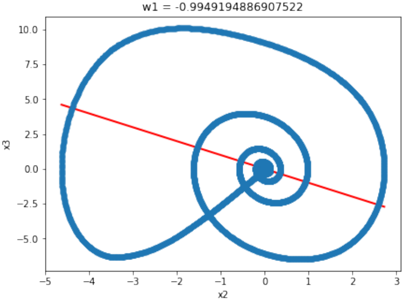
but what if we simply transform it so that a linear relationship holds?



System identification with linear regression

Applying linear regression to it, we can recover the length and damping coefficient!





Linear parameter models

Linear regression can be used to solve complex nonlinear problems, by transforming the data so that it is linear in some domain

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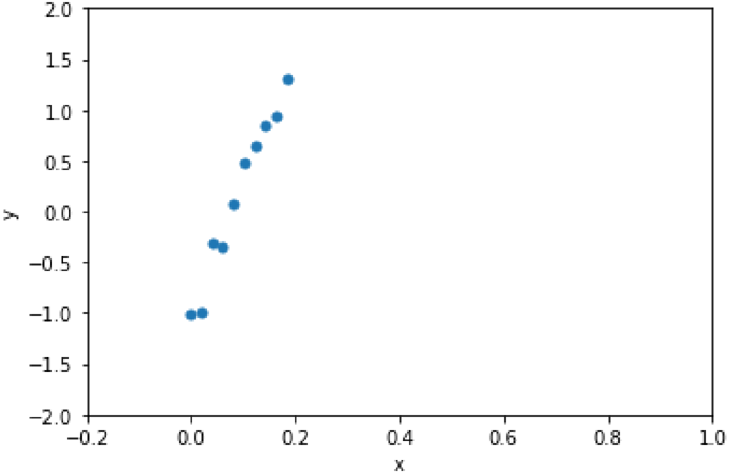
- we're only limited by our imaginations
- but life is not that simple...

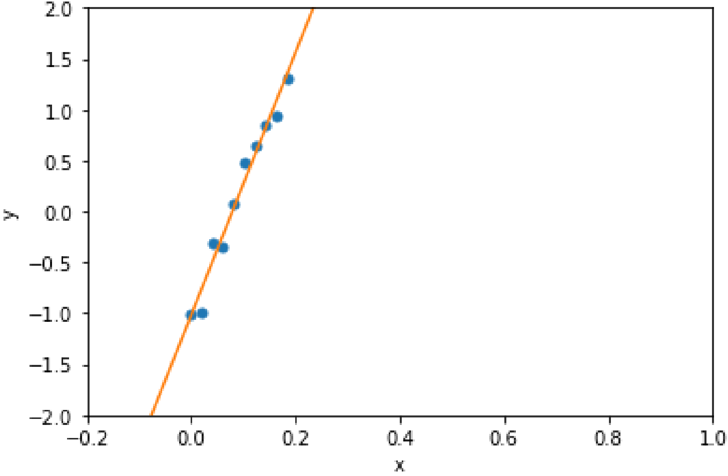
Polynomial expansions

Lets look at another example...



Polynomial expansions

Looks linear, so lets fit a linear model $\mathbf{y} = [1, \mathbf{x}]\mathbf{w}$



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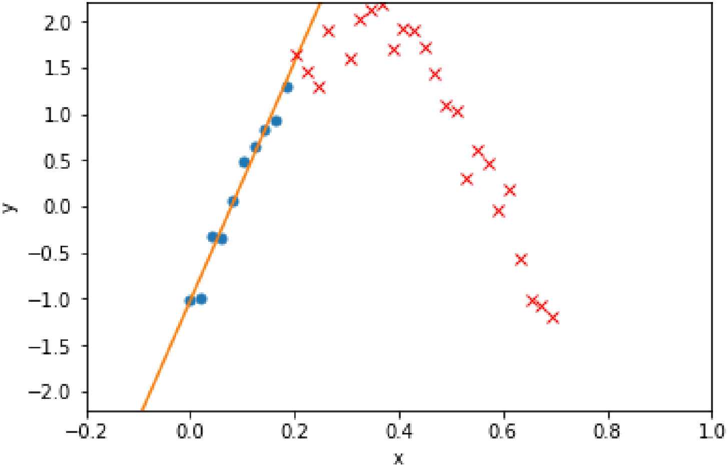

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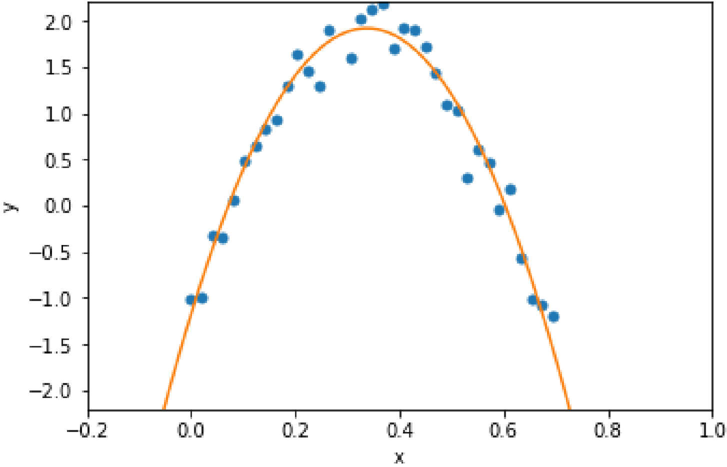

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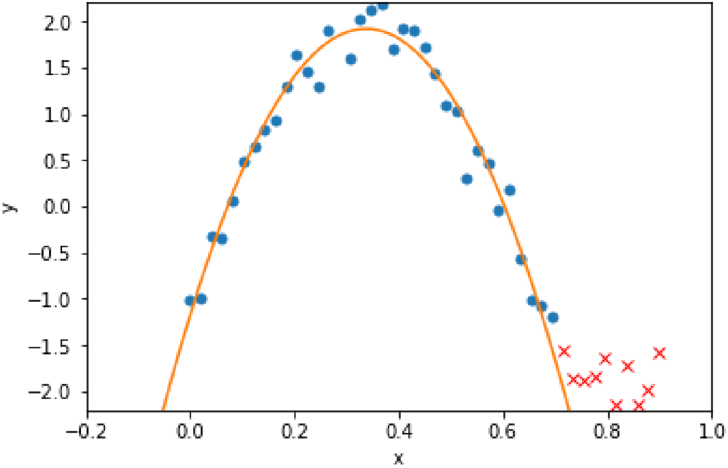

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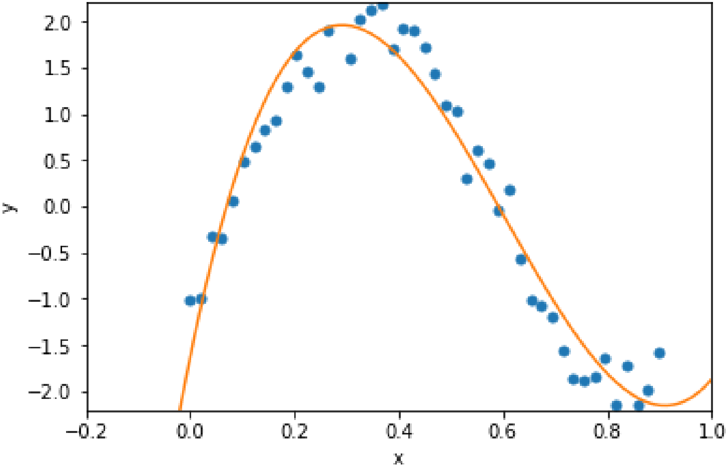
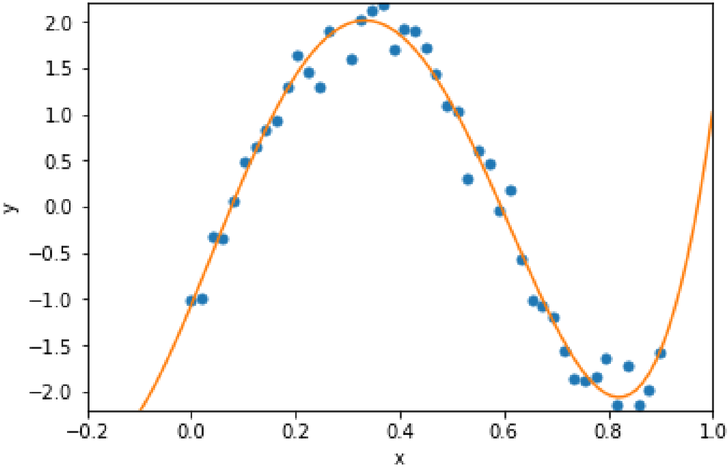


Polynomial expansions

and a fourth order...



Polynomial expansions

A few question arise:

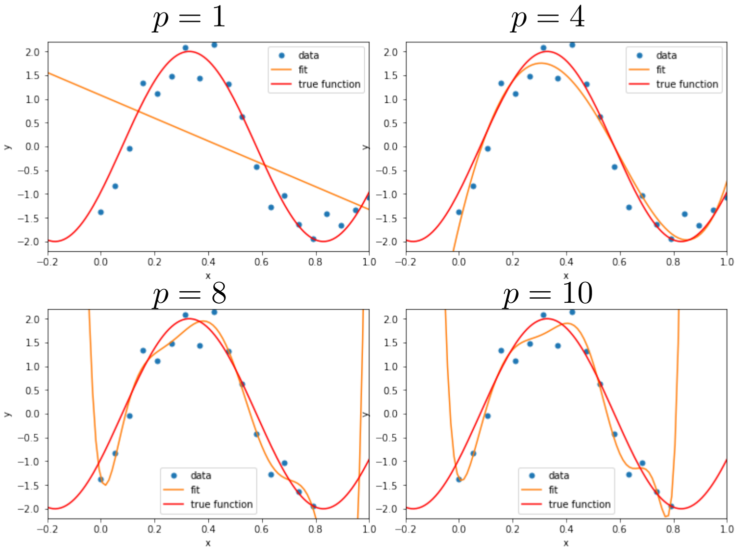
- Should we keep increasing the complexity of the models to minimise the training error?
- At what point do we stop?
- How do we assess model performance outside of the region covered by training data ?

Model Complexity

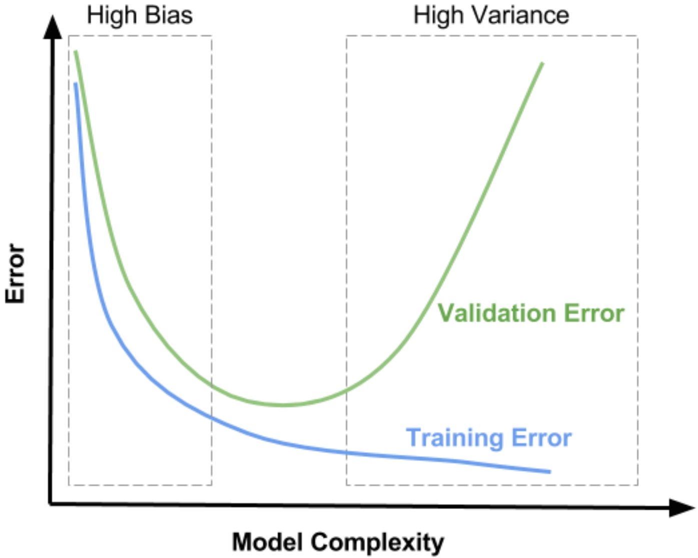
By now, we will have noticed that

- Simple models don't perform that well on complex data
- Complex models perform well on the data that they've been trained on, but fail to accurately predict outside that range. They **over-fit**

Bias, Variance and overfitting



Bias and variance



Bias and variance

- Simple models underfit / have high bias / high training error
- Complex models overfit / have high variance / high generalisation error
- A balance is needed!

Bias and variance

We have two main tools to balance model complexity and quality of fit:

- Regularisation
- Cross-validation

Regularisation

One way to achieve a balance of complexity and quality of fit is to penalise more complex models through additional terms in the loss function.

In linear regression, a popular penalty is:

$$J(\mathbf{w}) = ||\mathbf{y} - \mathbf{X}\mathbf{w}||_2^2 + \lambda||\mathbf{w}||_p \tag{1}$$

Note that this penalty can also be interpreted as a constraint on the loss function

Regularisation

$$J(\mathbf{w}) = ||\mathbf{y} - \mathbf{X}\mathbf{w}||_2^2 + \lambda||\mathbf{w}||_p \qquad (2)$$

The norm, p, in the loss function plays an important role on the type of regularisation.

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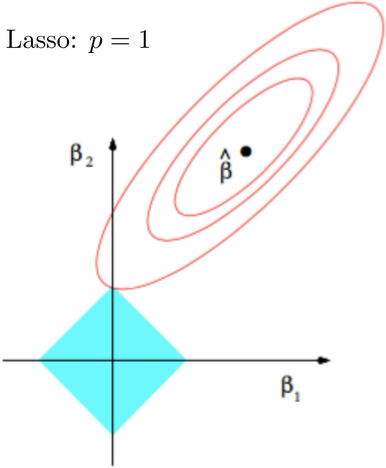
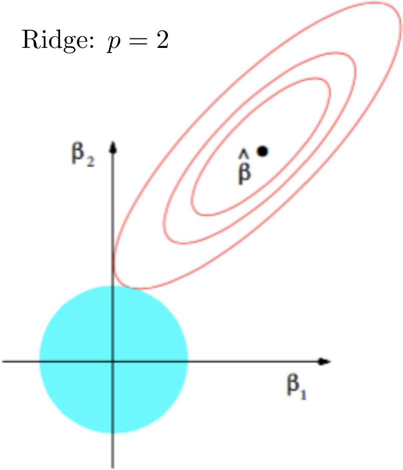
- We'll focus on $p = 2$ here, otherwise known as Tikhonov reugarisation

Regularisation constraints of Lasso and Ridge regression





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    - the bases/columns in $\mathbf{X}$ are not linearly independent (solution is not unique)

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- Our loss function has an additional term, $||\mathbf{w}||_2^2$
- and we have that $\nabla||\mathbf{w}||_2^2 = 2\mathbf{w}$

Deriving Tikhonov regularisation

We need to minimise:

$$J(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) + \lambda||\mathbf{w}||_2^2$$

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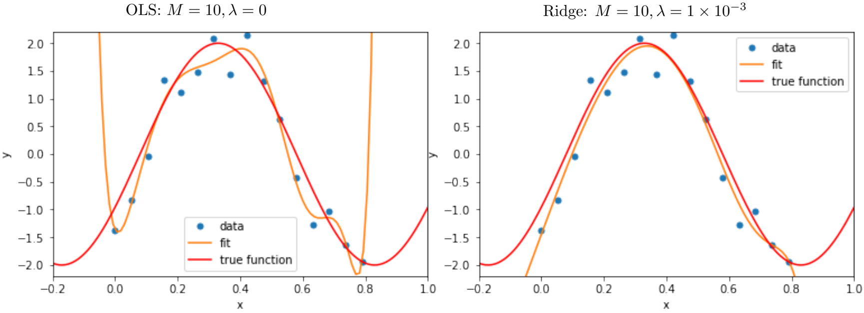
rearranging for $\mathbf{w}$

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Regularisation - Example



Regularisation

Life is good, but have we replaced one problem with another?

- The regularisation coefficient, λ now balances model complexity
- We need an effective method for selecting it, based on generalisation performance

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Conclusions

What have we learned today?

- How to do nonlinear regression, using linear regression
- Generalisation
- The bias-variance trade-off - balancing model complexity
- Regularisation

So... what next?

Tomorrow, we'll learn about some even more flexible models for regression, and how to tune hyper-parameters through cross-validation ;)