Week 4a:

Regularisation: Learning linear models that generalise

G6061: Fundamentals of Machine Learning [23/24]

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Outline

Today we'll

- Think about relaxing some of our assumption in **learning linear regression**.
- Discuss the concept of **over-fitting** and explain why it happens and how you can spot it.
- Introduce **regularisation** as a mechanism to combat overfitting, and explain it's link to Bayes' theorem.

At the end of this session you should be able to

- Understand how weighted least squares fitting works, why it can be useful, and how to implement it in `numpy`.
- Describe the concept of overfitting, and be able to spot if your model is overfitting.
- Explain what regularisation is, and how it can be applied to reduce overfitting.

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Recap: linear least squares regression

- We defined linear regression as:
  $y \approx \hat{y} = Xw$, where y=labels, $\hat{y}$ =prediction, X=input data matrix, and w=weight vector
- We defined the *cost function* as the squared prediction error:
  $\frac{1}{2N} \|X\mathbf{w} - \mathbf{y}\|^2$
- This gives us a *probabilistic interpretation* of our predictions as a normal distribution $\mathcal{N}(y; X\mathbf{w}, \sigma^2) = \mathcal{N}(y; \hat{y}, \mathbf{I}\sigma^2)$.
- This states: errors are independent & *identically distributed* across samples
  - Is this realistic? Can you think of a case when it wouldn't be?
  - How can we relax the assumption that the distribution of model errors is the same across samples?

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Weighted linear regression

- There are often times where assigning different weights on our training data pairs i.e. (x_n, y_n) might be helpful.
- This would be because we may have more or less confidence in some data points than others
  - For instance, maybe one of the hiring managers makes erratic decisions and we wanted to downweight their opinions.
  - Alternatively, another one might always make excellent decisions and we want to model that process.
- **Warning!** Blindly assuming our models are informative can exacerbate human bias and unfairness in decision making.
  - We're not covering AI fairness and bias in this module, but I'd recommend that you check out this blog post on the topic.

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Weighted linear regression

- We can modify linear least squares regression to allow σ^2 to change across training samples.
  - This is known as heteroscedastic noise.
- Our problem is *mostly* the same, we just attribute different importance to some of the data.
- Mathematically, we can still write it in *closed form*

$$\mathbf{w}^* = (X^\top W X)^{-1} X^\top W y$$

where W is a *diagonal matrix* containing the reciprocal sample variance $W_{ii} = \frac{1}{\sigma_i^2}$

```
# Given X, y and W
w_hat = np.linalg.inv(X.T@W@X)@X.T@W@y
# We can still use the psuedoinverse
w_hat = np.linalg.pinv(np.sqrt(W)@X)@np.sqrt(W)@y
y_hat = X@w_hat # predict
```

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How do I know what σ should be?

- Depends on your problem.
  - Sometimes you know the expected precision of a sensor
  - Or how erratic a human labeller is!
- You can also learn or infer it from data, but that's a more advanced use case.

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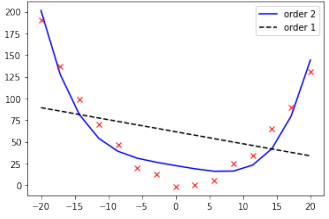
Making linear models complicated

- Last week we saw how linear models could be extended to explain more complex relationships in the input data.

$$X = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^K \\ 1 & x_2 & x_2^2 & \dots & x_2^K \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 & \dots & x_N^K \end{bmatrix}$$

So we can fit polynomials, or any set of basis functions:



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But what if our model is too complicated?

- What will it do?
- It will probably be better at describing the data you trained it on!
  - i.e. the training error will be lower.
- It will probably be worse at describing the unseen validation or test data!
  - Which means that practically speaking, it's not very useful!

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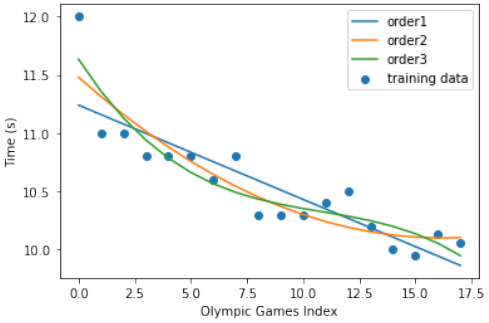
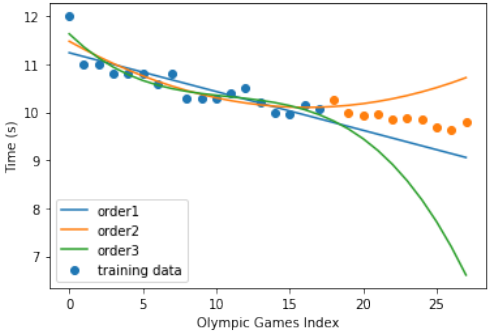
Polynomial regression





Sometimes the simplest model will be best for predicting new data.

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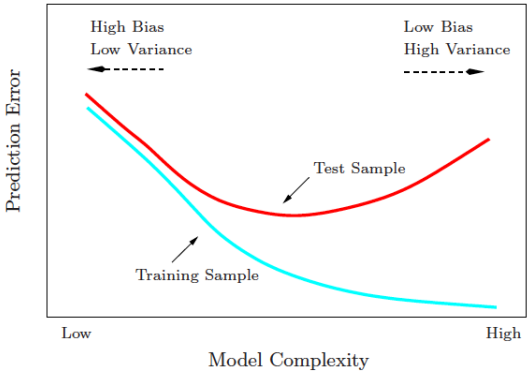
Training and test error as a function of model complexity

For example, the higher the degree of a polynomial, the more complex.



The Elements of Statistical Learning

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Think break

- Our linear model produces an output by

$$\hat{y} = \sum_i w_i x_i$$

- We can make the model more complicated by adding new variables to x, e.g.:

$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$$

- What *prior knowledge* could we build into our learning to make the model less complicated?
  - How can we make a complex model act like a simple model?

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Regularisation – intuition

- Consider the 5th order polynomial model

$$\hat{f}(x; \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$$

- Even if this model itself has 6 possible parameters to learn, we can simplify it in several ways.
- The most trivial model: $\mathbf{w} = (0, 0, 0, 0, 0, 0)$, and the model will always predict a value of zero.
- The next simplest model: set w_0 **to some non-zero value**, and the model will predict a constant w_0.
- The next next simplest model: **leave** w_0 **at its new value**, we can **set** w_1 **to some value**. The model has become more complex, it can predict a line now!

Regularisation and model complexity

- The 5th order polynomial model has more available complexity as we allow each additional parameter w_n to be given a non-zero value!
- One way to think of this, is the more non-zero weights, the more complex the model. $||\mathbf{w}||_0$
  - The L^0 norm is **not** differentiable, as it's a count, so tricky to optimise dynamically.
- Another description of complexity is: the more $\mathbf{w}$ deviates from 0, the more complex the model is.
  - This can be written as the **sum of absolute values**, $L^1 = ||\mathbf{w}||_1$.
  - But absolute value tend to be tricky to optimise, as it's not differentiable at 0.
- What might we use instead?

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Another squared term

- A squared term is helpful again.

$$||\mathbf{w}||_2^2 = \sum_{i=0}^{d} w_i^2$$

or, in a vector form,

$$\mathbf{w}^\top \mathbf{w}$$

- This gives us a description of model complexity that increases as the square of the weight values.
- Where do you think this might have come from?

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The Gaussians are back!

- Again, the squared term comes from a Gaussian/Normal distribution! which has a log-probability $\log p(\mathbf{w}|\mu, \sigma^2) \propto \frac{(\mathbf{w}-\mu)^\top(\mathbf{w}-\mu)}{\sigma^2}$
  - in our case $\mu = 0$
- But this time we can think of it slightly differently, and see this as a *prior* distribution on the values of $\mathbf{w}$.
  - This means it expresses our preferences on what values $\mathbf{w}$ should take, before we've seen any data.
  - Instead of σ^2 describing noise, it's describing the *flexibility* that we're giving our model to choose various values for $\mathbf{w}$. As our preference is for $\mathbf{w}$ to be 0, we set $\mu = 0$ for most cases.

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Maximum Likelihood

- When we discussed linear regression, we expressed it probabilistically saying our signal was corrupted with Gaussian noise.

$$p(\mathbf{y}|\mathbf{x}, \mathbf{w}) = \mathcal{N}(\mathbf{y}|\mathbf{x}^\top \mathbf{w}, \sigma^2)$$

- This equation is the *likelihood* of observing $\mathbf{y}$ given that we've seen $\mathbf{x}$ and $\mathbf{w}$.
- When we found the best values of $\mathbf{w}$ before, we were doing Maximum Likelihood estimation!

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Maximum-A-Posteriori

- Now we're adding regularisation as a prior distribution, we're actually doing a form of *Bayesian inference!*
- Bayes' rule can be written as:

$$p(\mathbf{w}|\mathbf{x},\mathbf{y}) \propto p(\mathbf{y}|\mathbf{x},\mathbf{w})p(\mathbf{w})$$

- taking logs on both sides

$$\log \underbrace{p(\mathbf{w}|\mathbf{x},\mathbf{y})}_{posterior} \propto \log \underbrace{p(\mathbf{y}|\mathbf{x},\mathbf{w})}_{likelihood} + \log \underbrace{p(\mathbf{w})}_{prior}$$

- So by *adding* the 2 log probabilities together and optimising that, we are finding the best values for $\mathbf{w}$ after seeing the prior and the data.
- This is called the *posterior* and finding the best value for $\mathbf{w}$ is called *Maximum-a-posteriori*.

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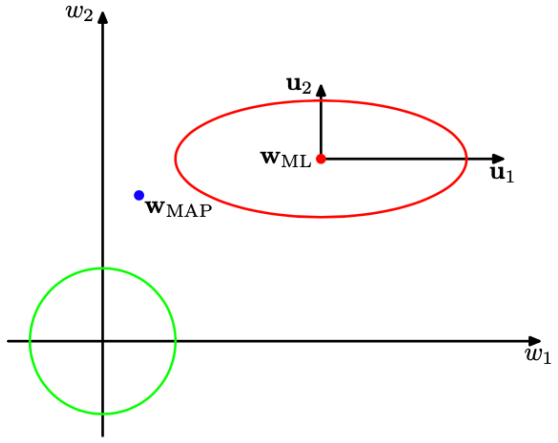
MAP vs. ML



A geometric perspective. w_{map} is between w_{ml} and the prior.

Taken from Bishop: Pattern recongition and machine learning

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Regularisation

- So rather than just minimising a loss function $\mathcal{L}(y, \hat{f}(x; \mathbf{w}))$, for example our residual error $\frac{1}{2N} \sum_{n=1}^{N} (y^n - \hat{f}(x^n; \mathbf{w}))^2$.
- We can minimise a **regularised** loss $\mathcal{L}'$ by adding together our loss $\mathcal{L}$ and a term penalising over-complexity:

$$\underset{\mathbf{w}}{\text{minimise}} \quad \mathcal{L}'(y, \hat{f}(x; \mathbf{w})) = \underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

  The **free (hyper-)** parameter $\lambda = \frac{1}{\sigma^2}$ controls the trade-off between penalising not fitting the data well ($\mathcal{L}$) and penalising overly complex models ($\mathbf{w}^\top \mathbf{w}$)
- Now we have
  - Regularised linear regression: $\mathcal{L}' = \mathcal{L}_{\text{squared loss}} + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w}$
  - Regularised logistic regression: $\mathcal{L}' = \mathcal{L}_{\text{logistic loss}} + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w}$
  - Regularised . . .: $\mathcal{L}' = \mathcal{L}_{\ldots} + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w}$

Regularised linear regression

$$\mathcal{L}' = \underbrace{\frac{1}{2N}\langle X\mathbf{w}-\mathbf{y}, X\mathbf{w}-\mathbf{y}\rangle}_{\text{residual error (see linear regression ecture)}} + \frac{\lambda}{2}\underbrace{\mathbf{w}^\top\mathbf{w}}_{\text{penalty term}}$$

Taking partial derivatives of $\mathcal{L}'$ with respect to $\mathbf{w}$ and set it to zero

$$\nabla_{\mathbf{w}}\mathcal{L}' = \frac{1}{N}X^\top(X\mathbf{w}-\mathbf{y}) + \lambda\mathbf{w} = 0$$

The regularised linear regression solution is

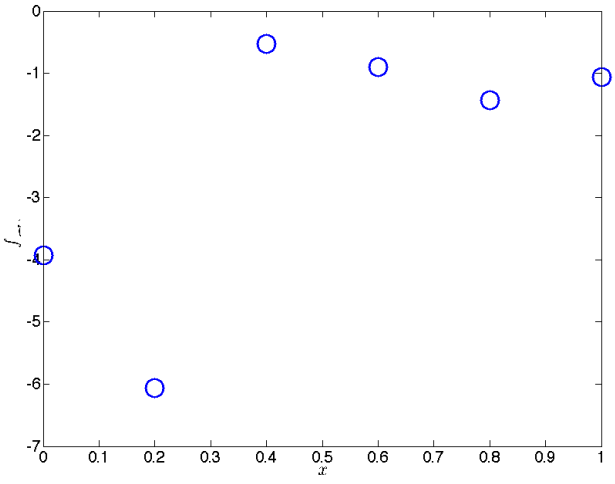
$$\mathbf{w}_{\text{regularised}} = (X^\top X + N\lambda I)^{-1}X^\top\mathbf{y} \quad \text{where } I = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}\Bigg\}$$

To be contrasted to our **non**-regularised version of linear regression

$$\mathbf{w}_{\text{non-regularised}} = (X^\top X)^{-1}X^\top\mathbf{y}$$

Regularisation in action

Our data with just 6 data points: $(0, -4), (0.2, -6), \ldots$



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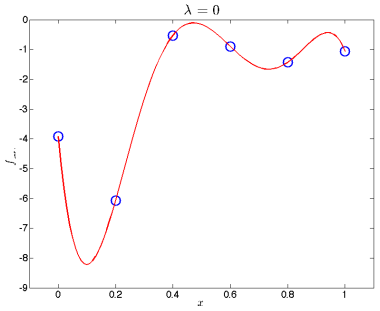
Regularisation in action

- We use the 5th order polynomial model

$$\hat{f}(x; \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$$

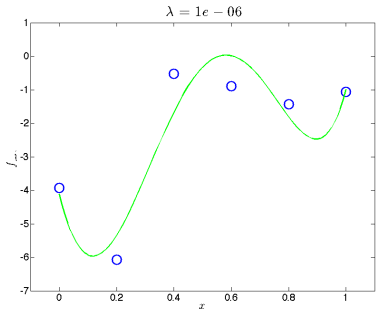
- We set $\lambda = 0 \rightarrow$ we recover the **non**-regularised version of linear regression



$$\underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

Regularisation in action

- We set $\lambda = 1e-06 \rightarrow$ the model follows the general shape of the exact 5th order polynomial but without as much variability and is further away from the data points.



$$\underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

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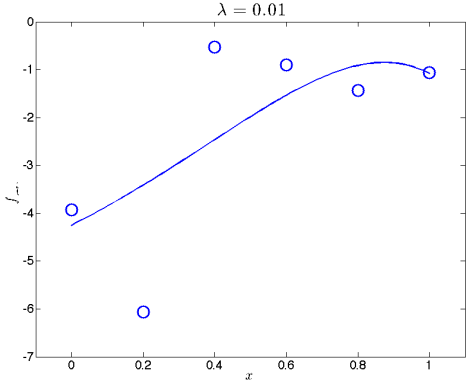
Regularisation in action

- We set $\lambda = 0.01 \rightarrow$ the model becomes less complex.



$$\underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

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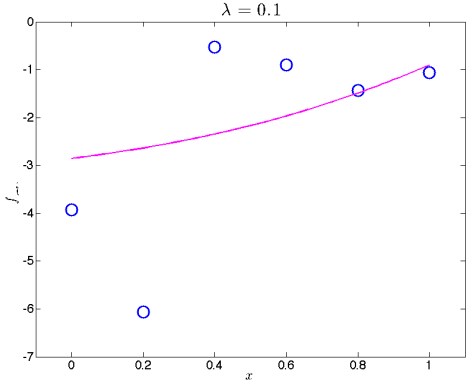
Regularisation in action

- We set $\lambda = 0.1 \rightarrow$ the model becomes even less complex.



$$\underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

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Regularisation in summary

$$\underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

- **Larger** λ, higher regularisation:
  too large, we will not capture any useful trends in the data

- **Smaller** λ, lower regularisation:
  too small, our function will likely be too complex

More regularization tends to cause less overfitting.

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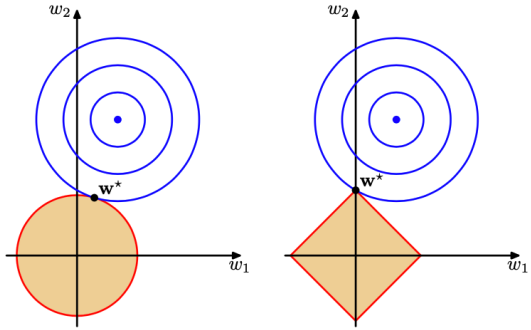
Other forms of regularisation

- LASSO (Least Absolute Shrinkage and Selection Operator) regularisation places a penalty on the absolute values of the weights $||\mathbf{w}||_1 = \sum_i |\mathbf{w}_i|$.



- Elastic net combines ridge regression and LASSO: $\lambda_1||\mathbf{w}||_1 + \lambda_2||\mathbf{w}||_2$
  - you need to balance the two terms though.

Taken from Bishop: Pattern recongition and machine learning

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Regularised linear models in sklearn

- Several options available in the sklearn.linear_models.
- Please investigate the documentation.
- Some regularisation types may use alternative optimisation approaches, and be much slower.

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Summary and outlook

- We've talked about how to incoporate how much we trust particular data samples in fitting linear regression.
- We've also introduced the concept of over-fitting, which we want to avoid.
- Finally, we covered *regularisation*, which enables us to encourage our models to be simpler.

Next lecture:

- We're still missing how to choose our hyper-parameters λ!
- Next time we'll cover Model selection: how to choose the model and it's hyper-parameters from data.

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