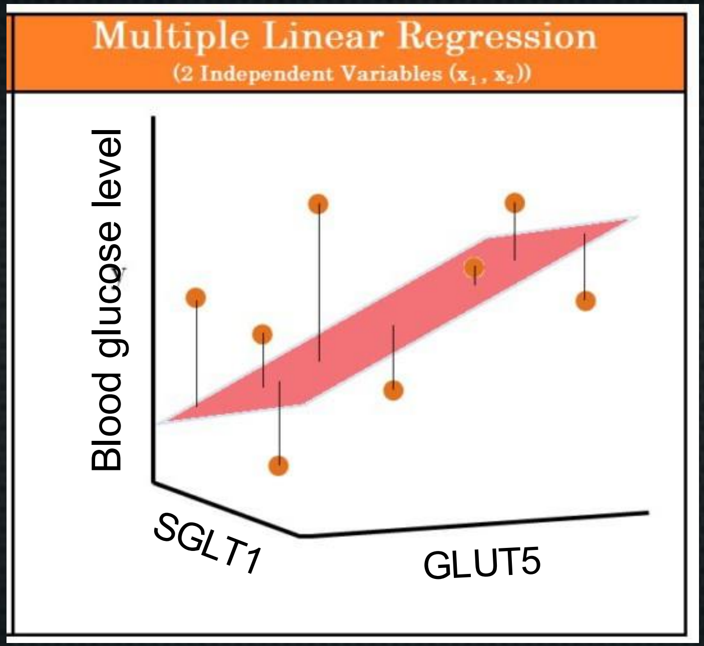
This presentation

- Adding multiple variables to your linear regression
- Why feature scaling is important
- Bias and variance: how do we make sure what we learn generalises?
- Cross-validation
- Learning curves

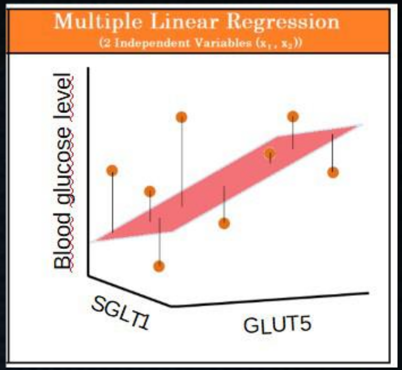
Multiple variables



Multiple variables

- Simple:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$



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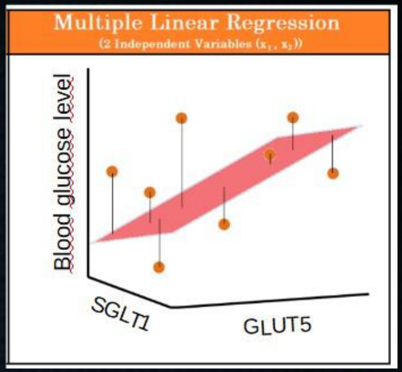

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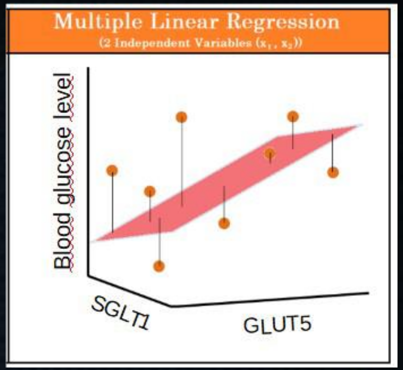
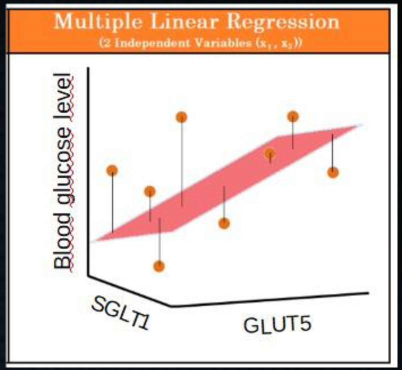


- Simple:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

$$J(\theta_0, \theta_1, \ldots, \theta_n) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x) - y^{(i)})^2$$

Multiple variables



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$$\theta_0=\theta_0-a\frac{\partial}{\partial\theta_0}J(\theta_0,\theta_1,\theta_2,\ldots,\theta_n)=\theta_0-\frac{a}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)})-y^{(i)})$$

$$\theta_1=\theta_1-a\frac{\partial}{\partial\theta_1}J(\theta_0,\theta_1,\theta_2,\ldots,\theta_n)=\theta_1-\frac{a}{m}\sum_{i=1}^{m}((h_\theta(x^{(i)})-y^{(i)})\cdot x_1^{(i)})$$

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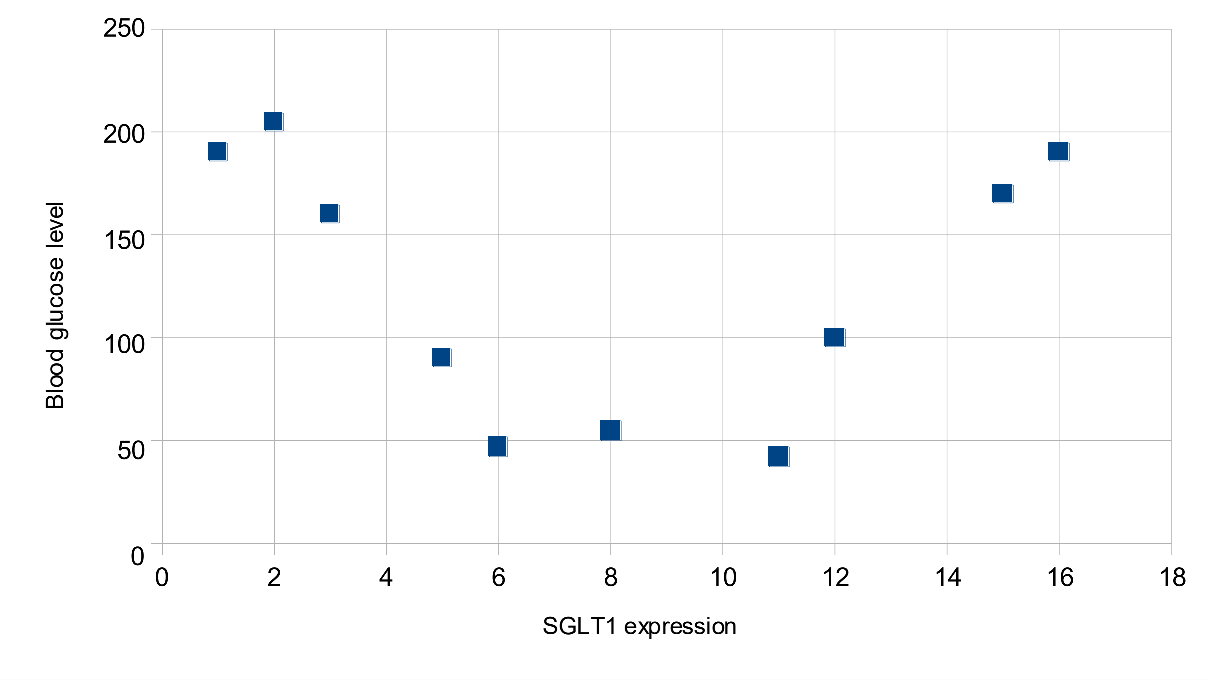
$$\theta_n=\theta_n-a\frac{\partial}{\partial\theta_n}J(\theta_0,\theta_1,\theta_2,\ldots,\theta_n)=\theta_n-\frac{a}{m}\sum_{i=1}^{m}((h_\theta(x^{(i)})-y^{(i)})\cdot x_n^{(i)})$$

Polynomials/power functions



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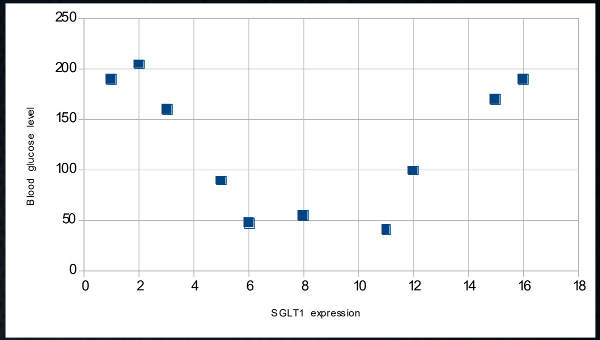

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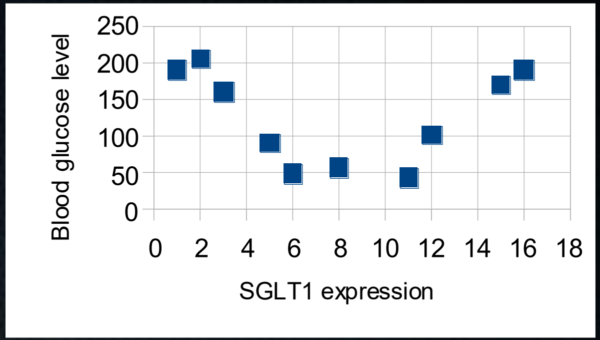

Sample #	SGLT1_linear (x1)	Blood glucose level (mg/dL)
1	3	155
2	8	55
3	12	101
4	2	200

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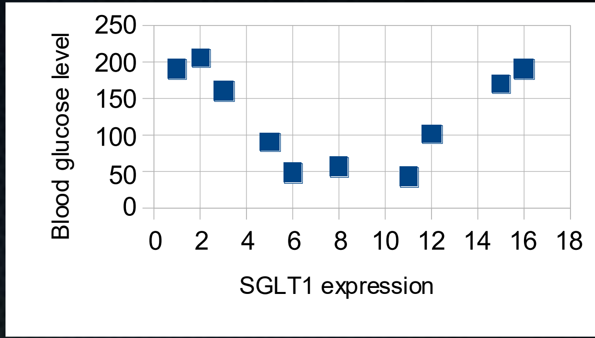

Sample #	SGLT1_linear (x1)	SGLT1_square (x2)	Blood glucose level (mg/dL)
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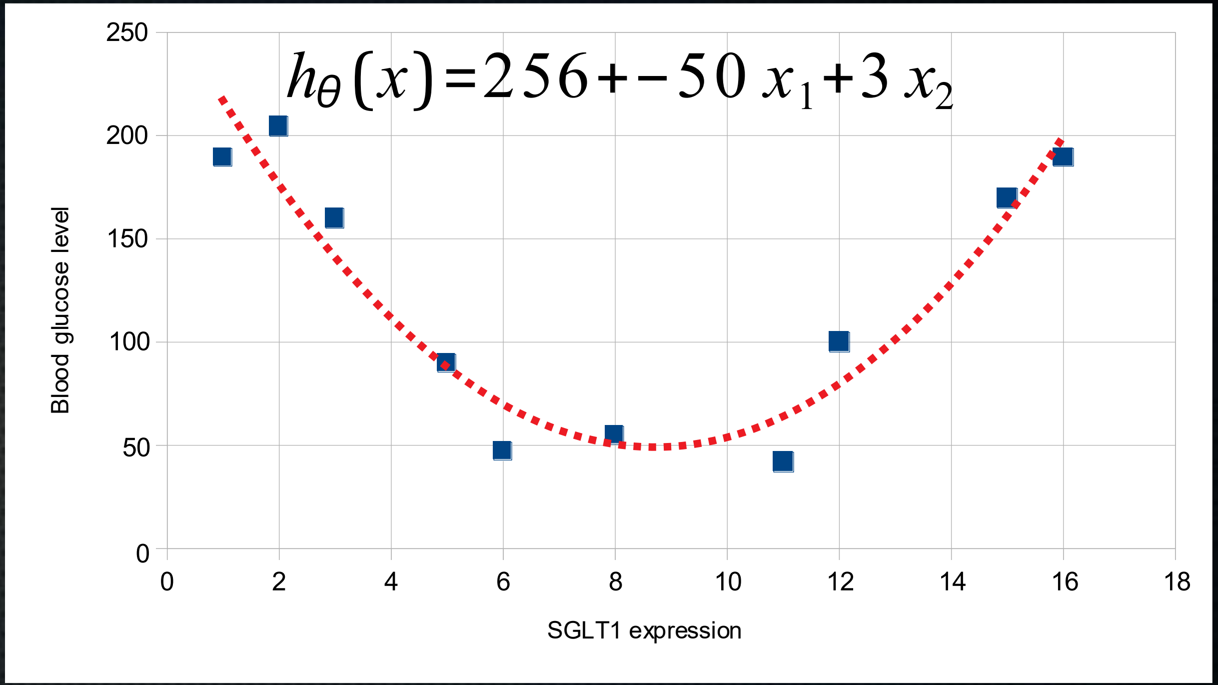

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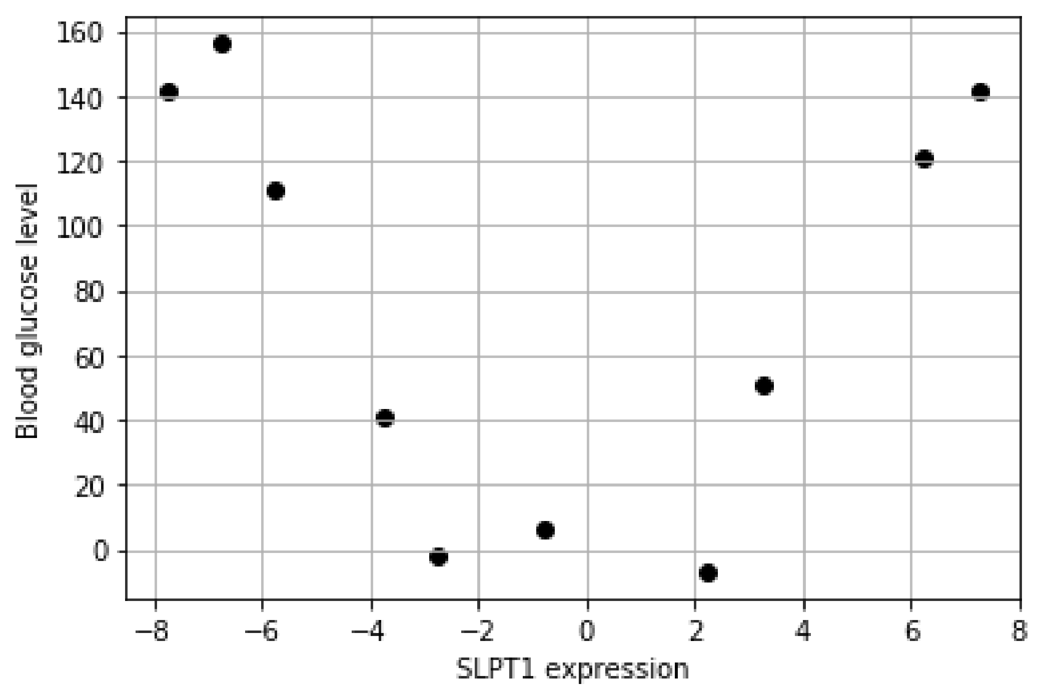

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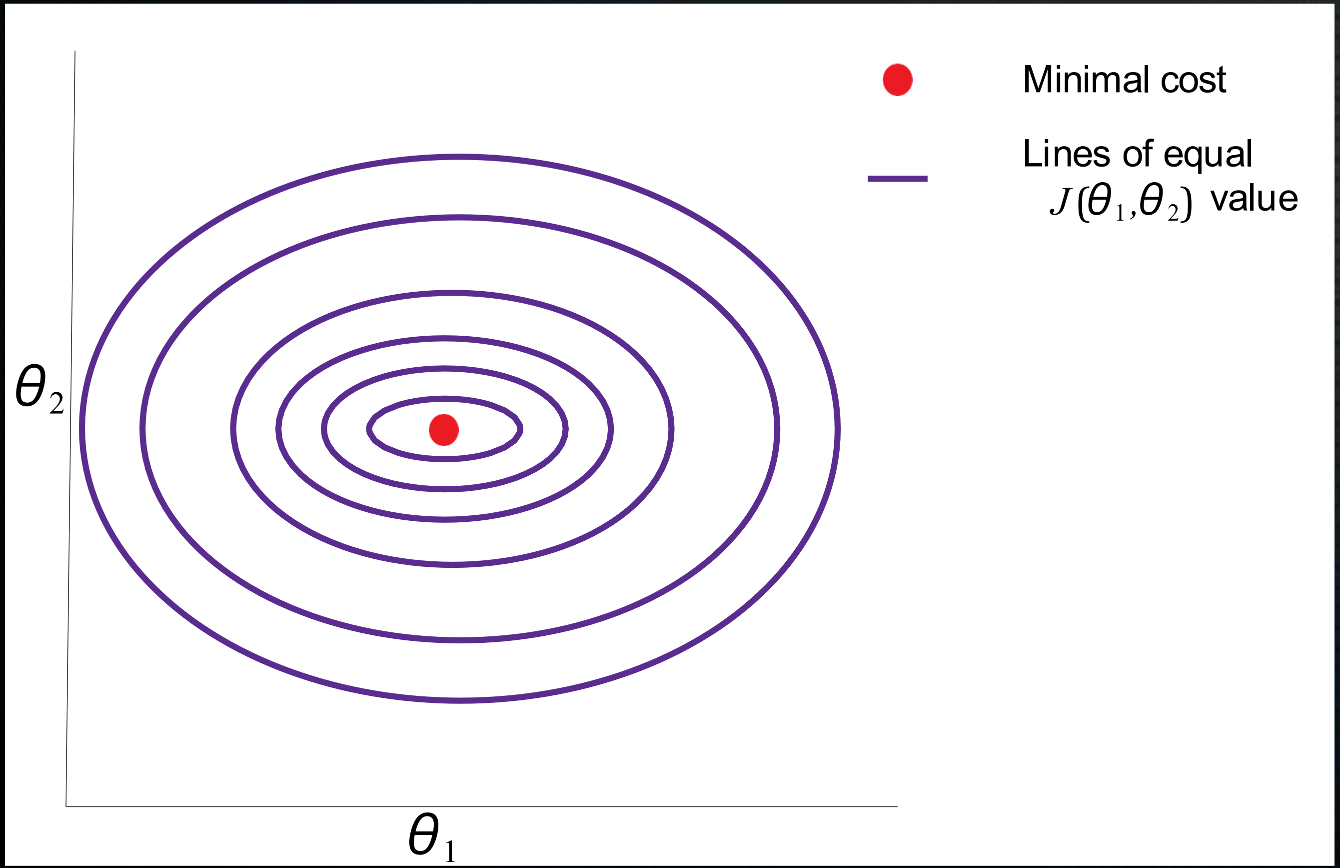

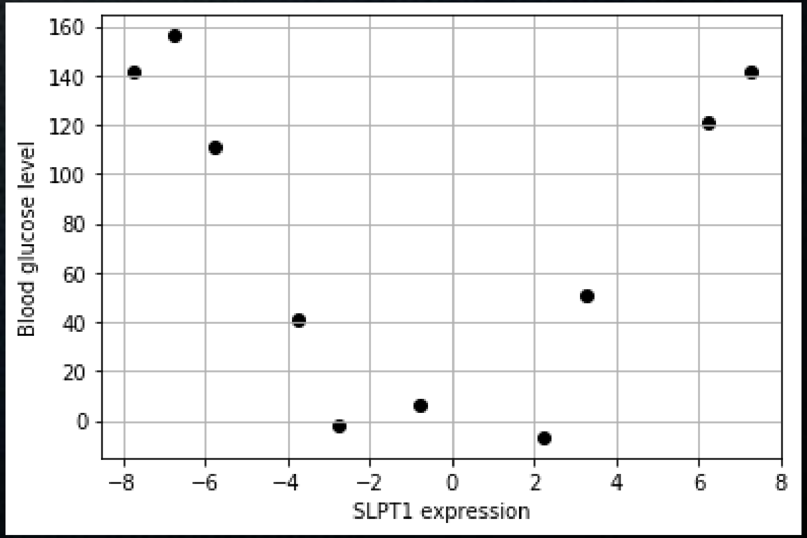

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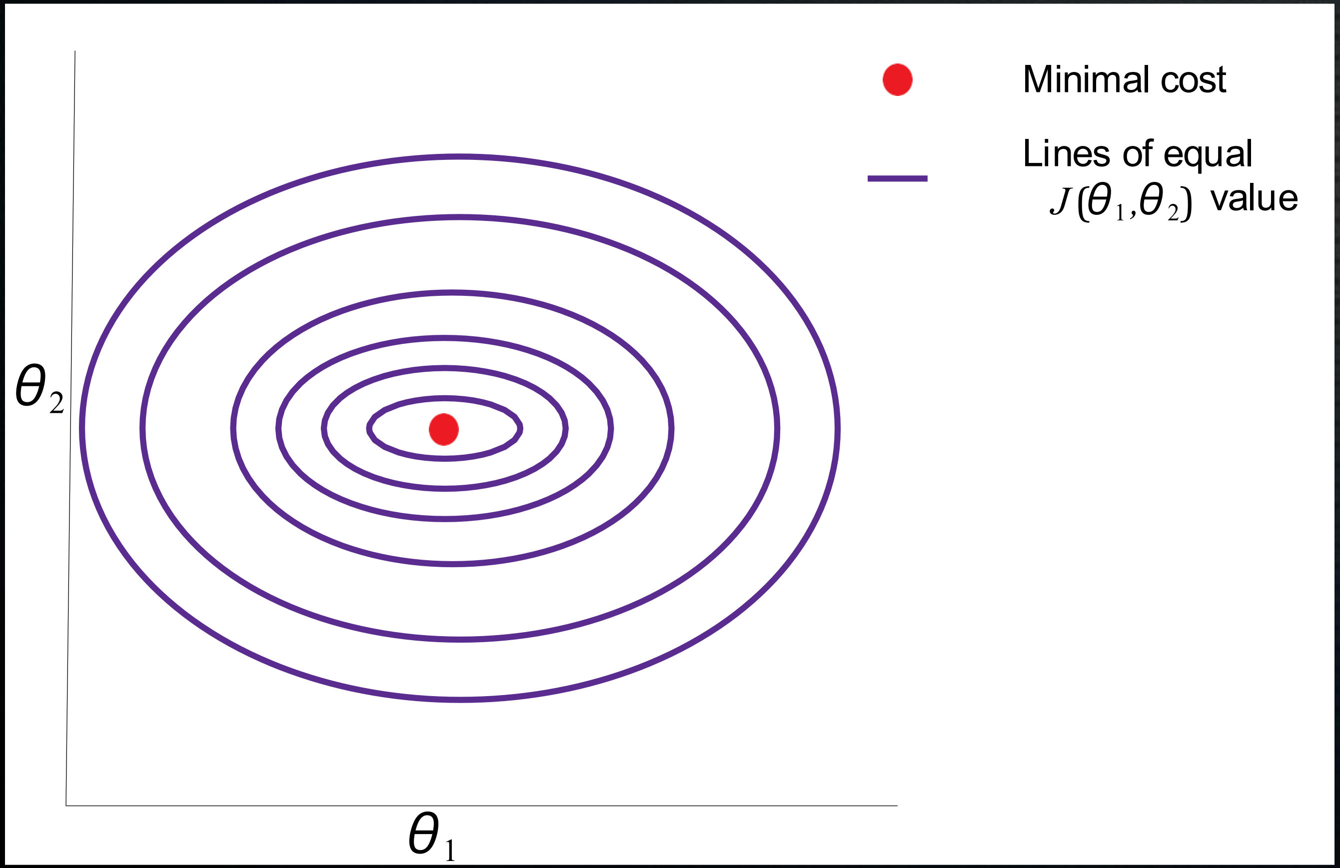

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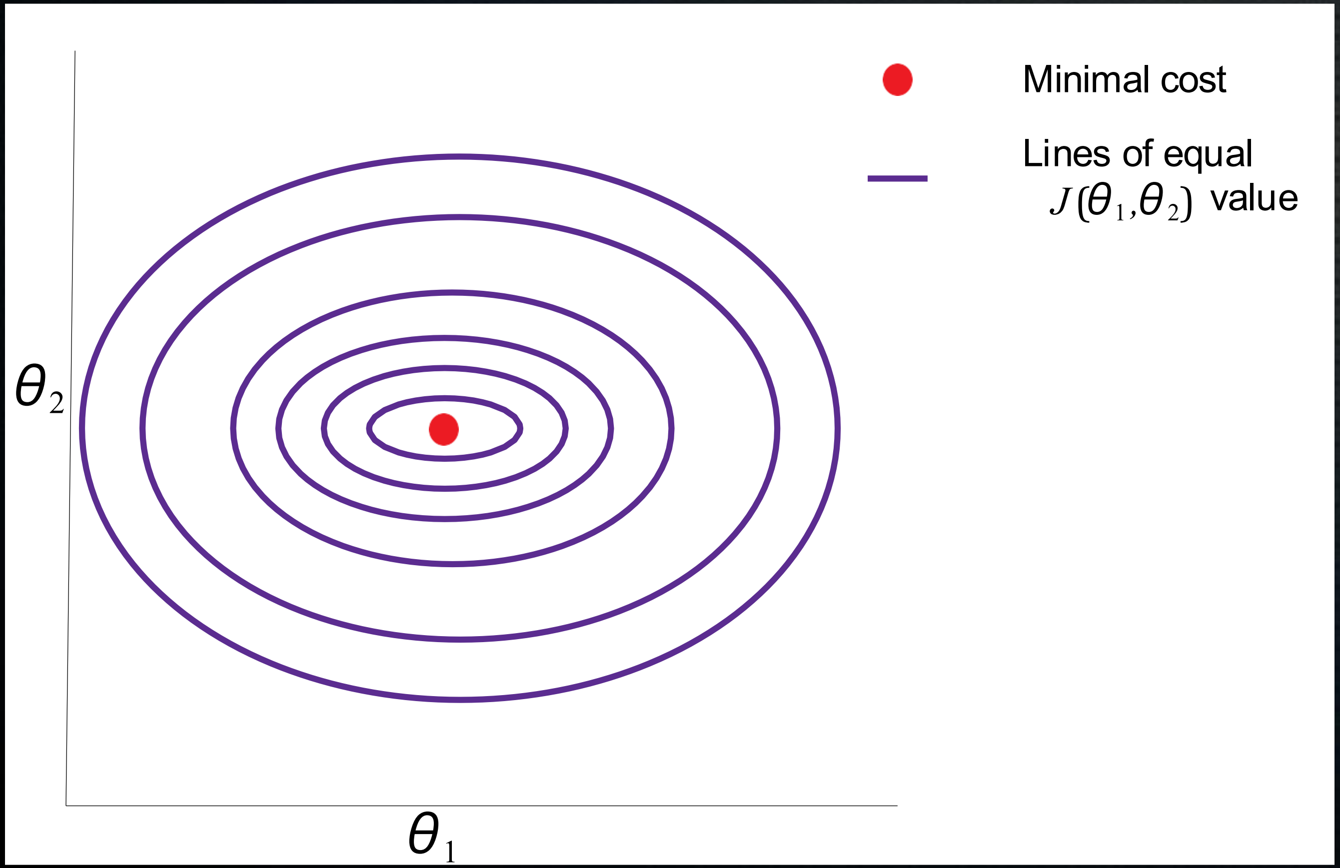

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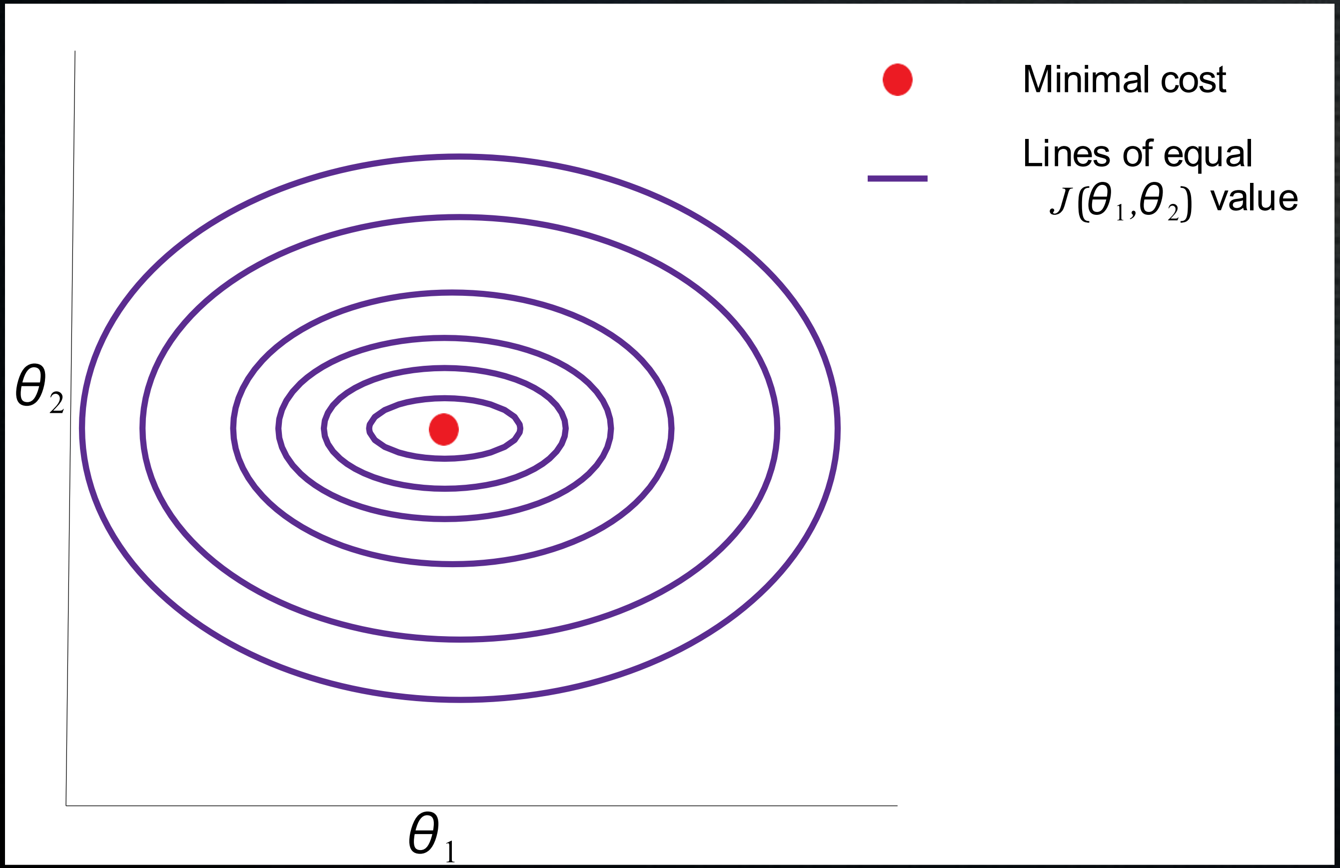

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Large steps

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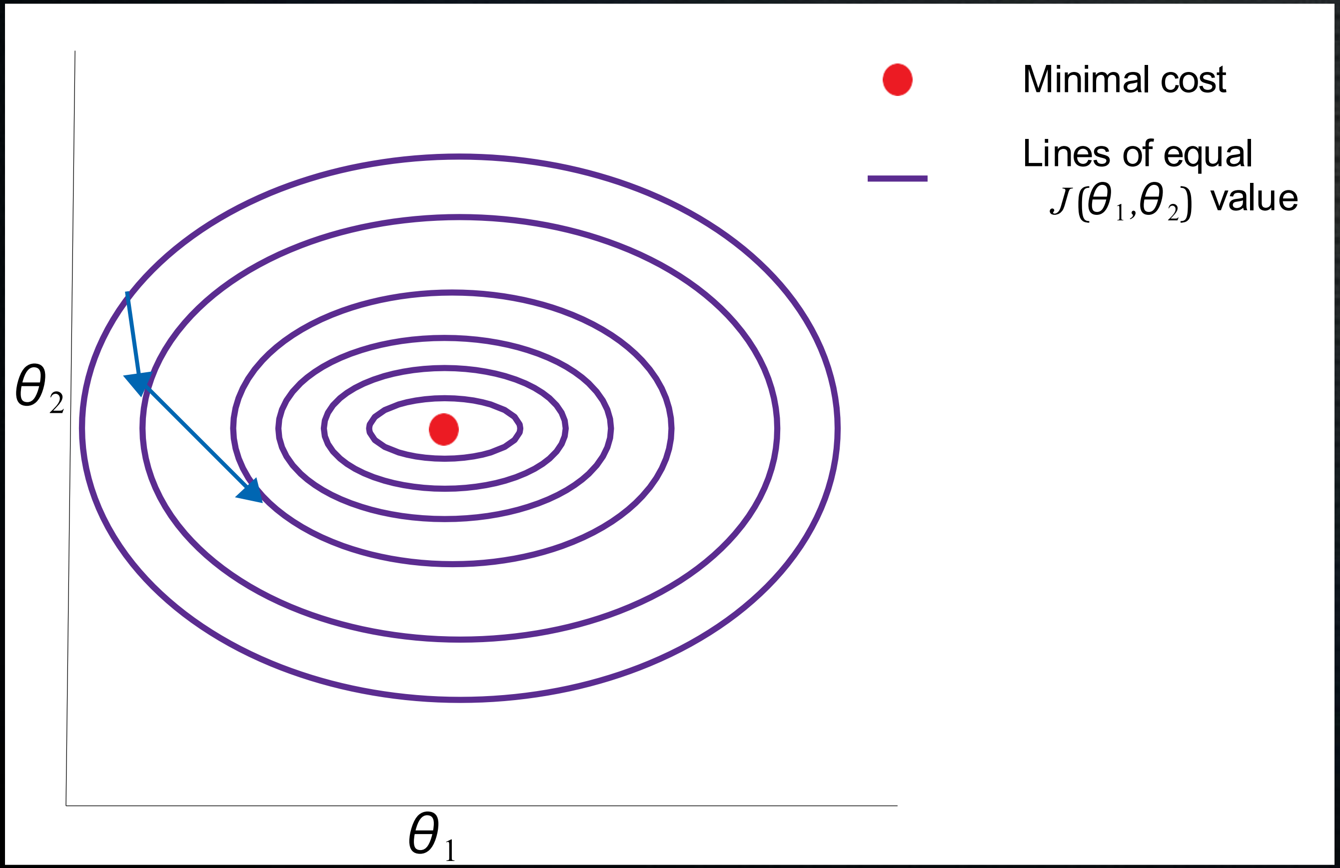

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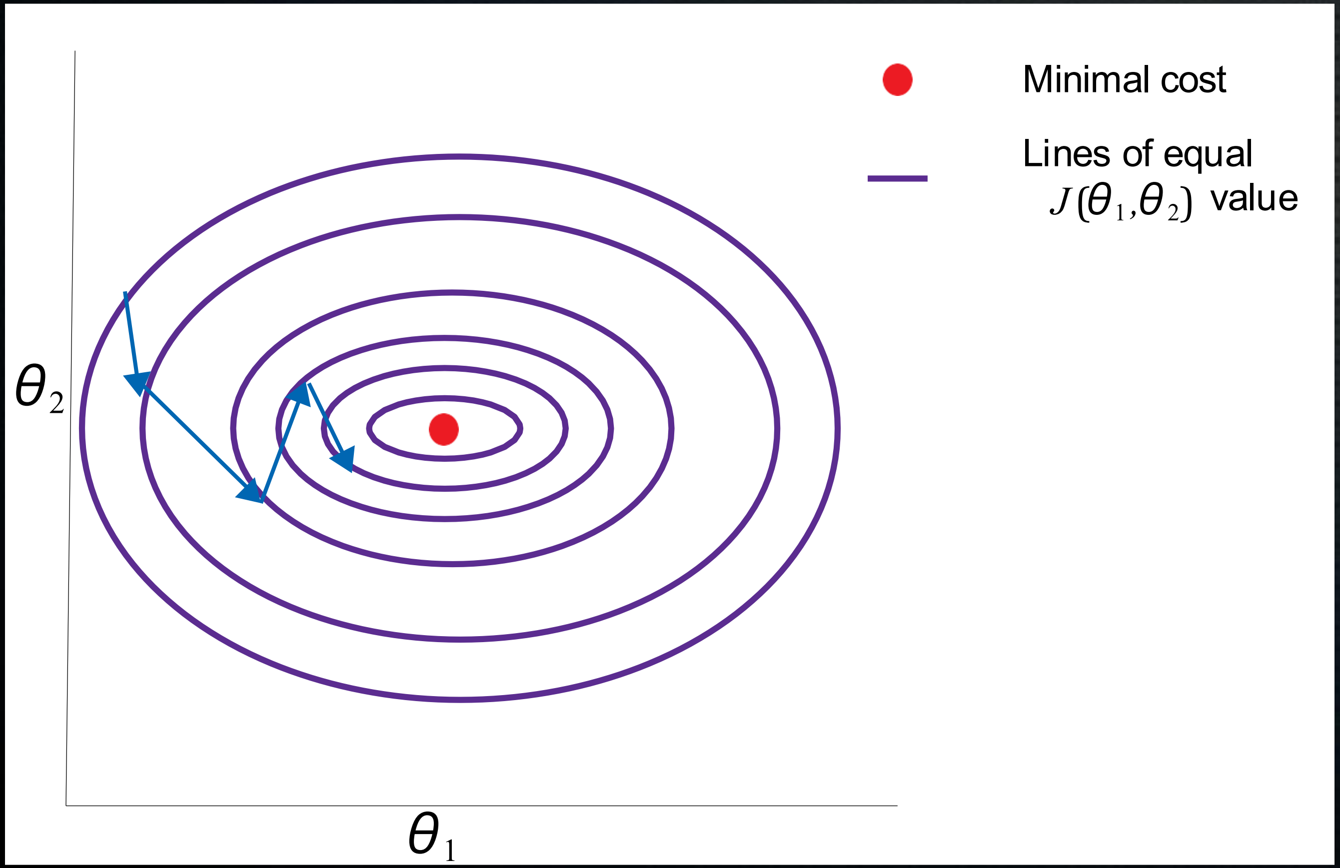

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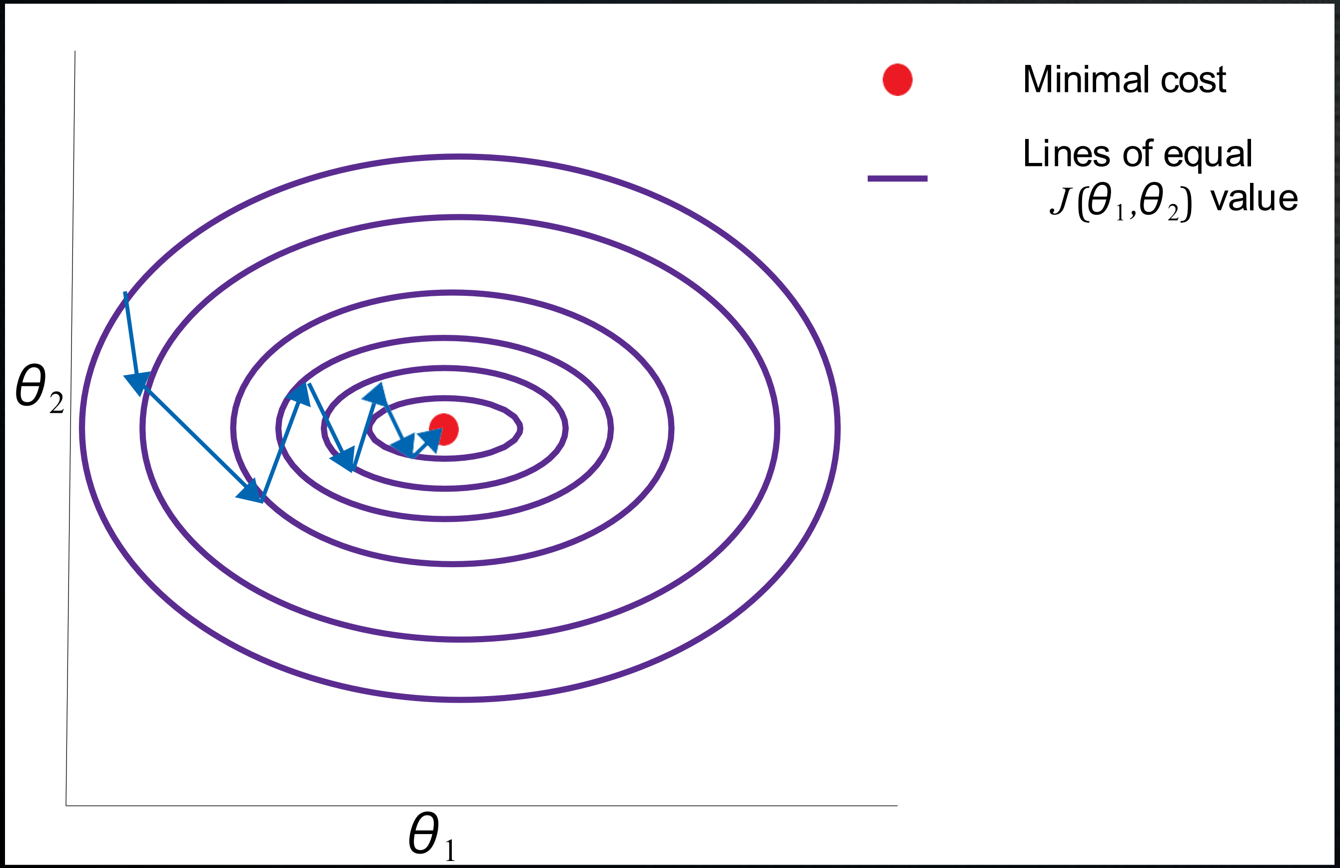

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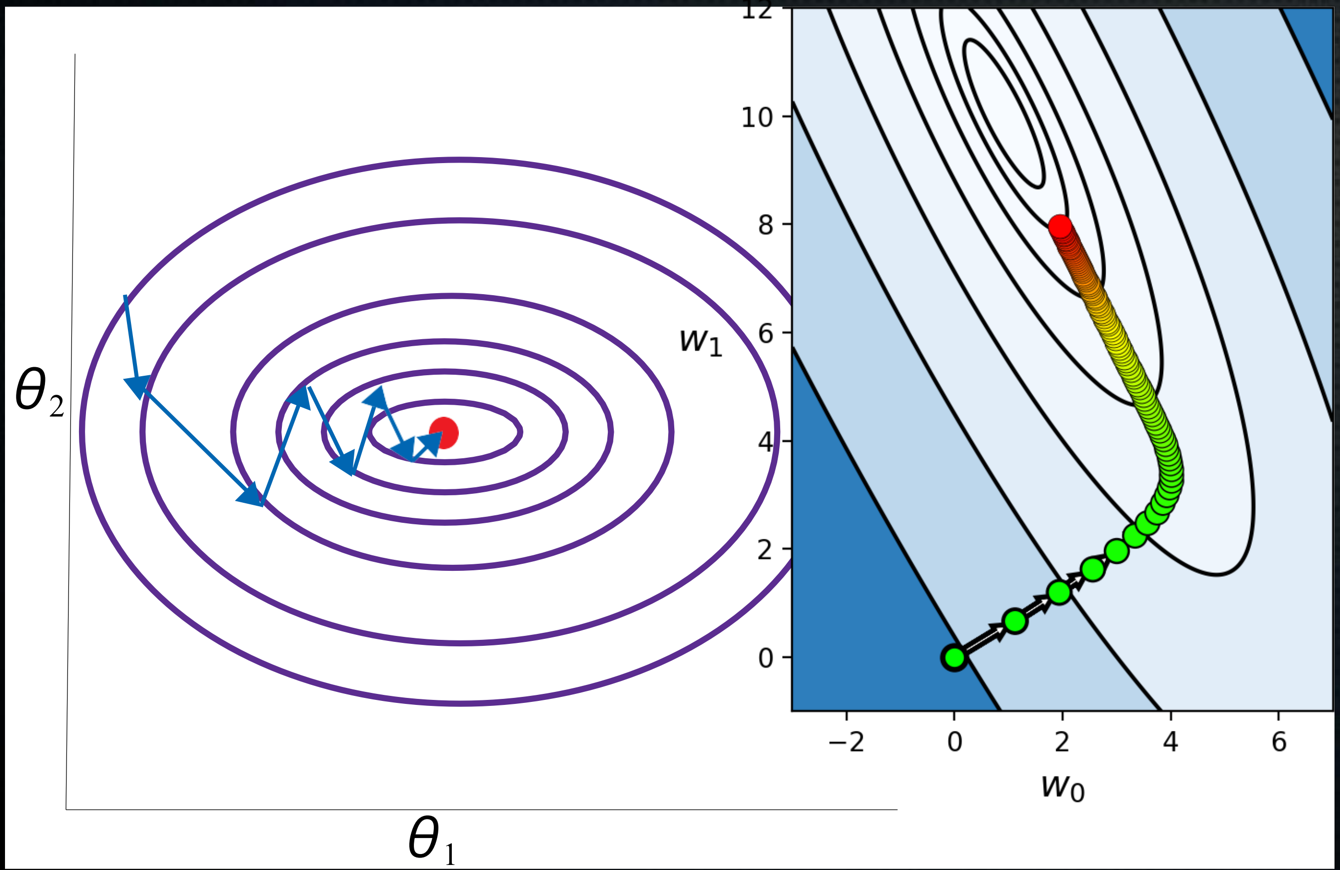

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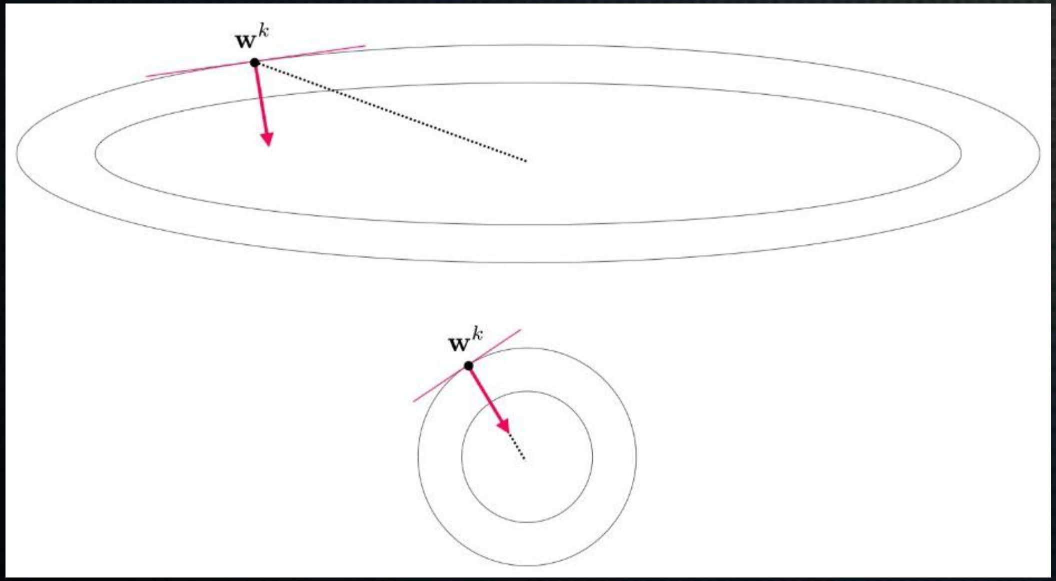

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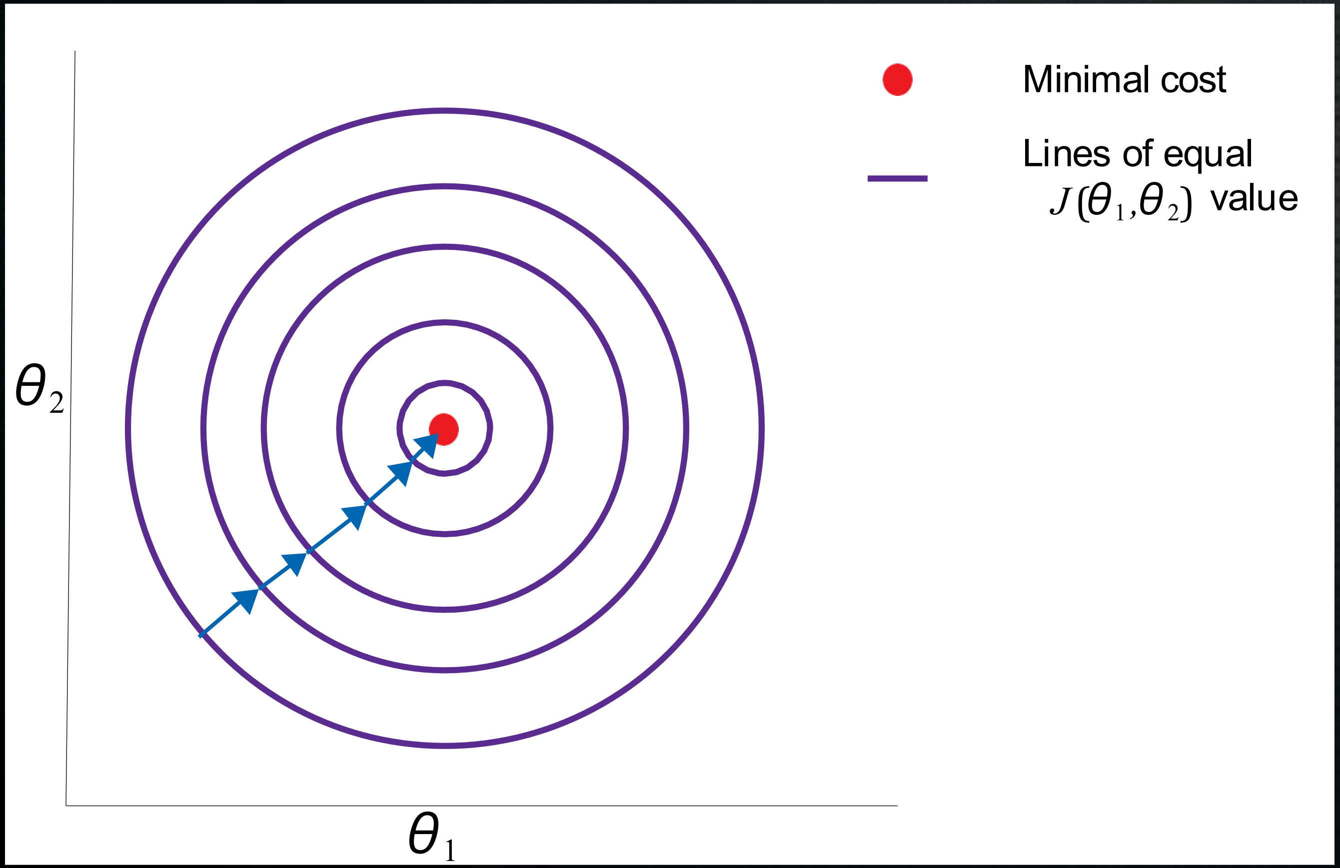

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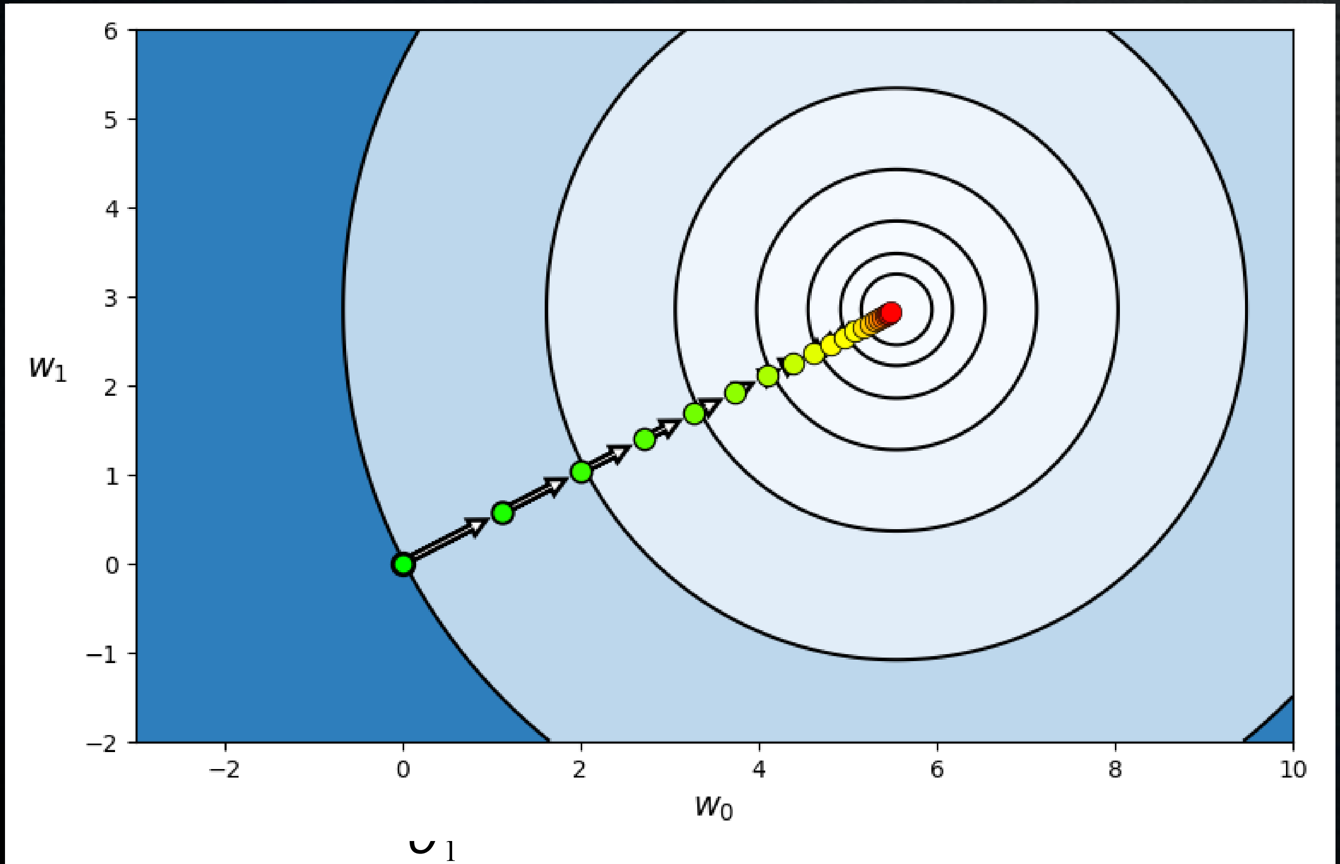
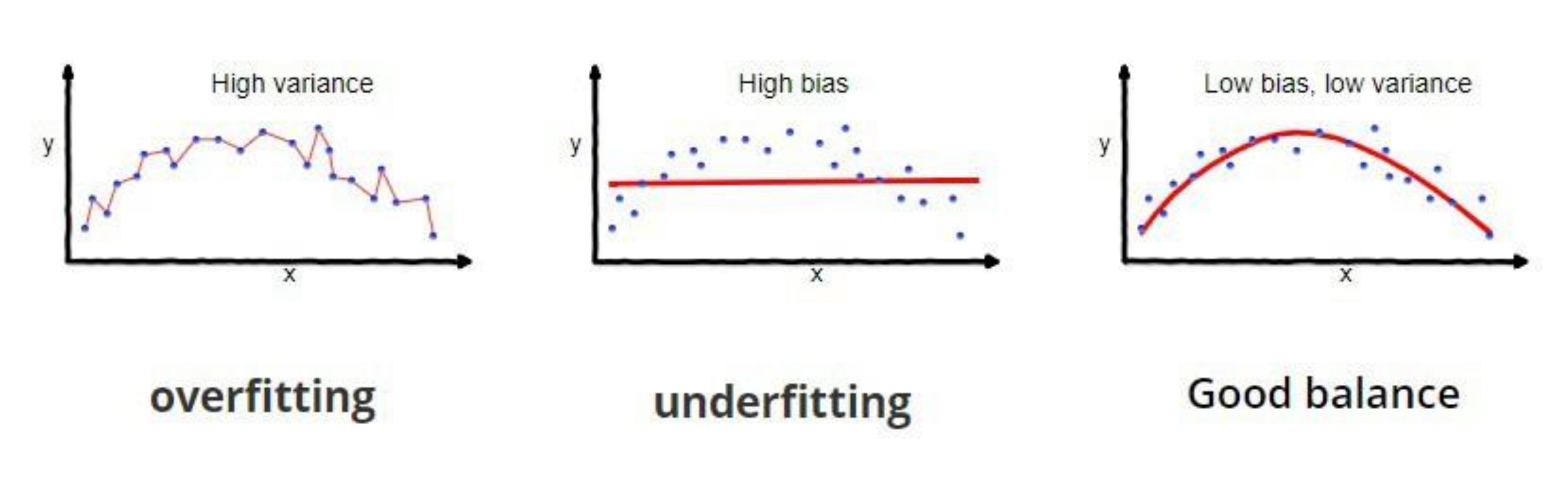


Summary

- Easily extendable to multiple features and polynomials
- Normalisation to help gradient descent converge faster

How to generalise well

- Goal is not to fit the training data perfectly, but to generalise well



Source: https://towardsdatascience.com/understanding-the-bias-variance-tradeoff-165e6942b229

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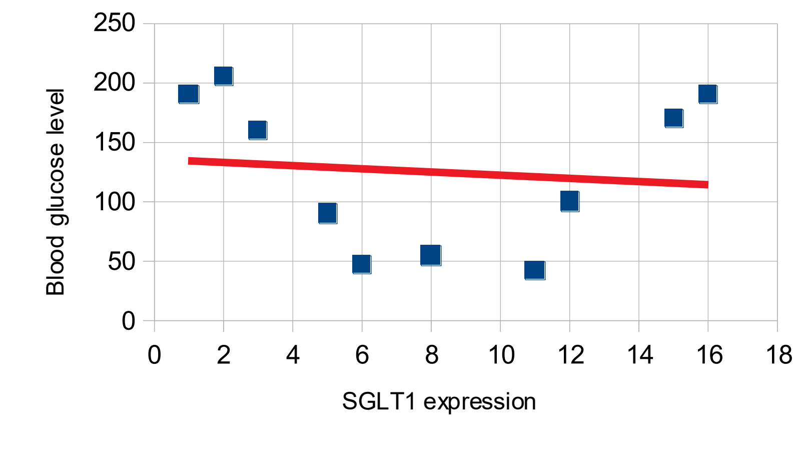

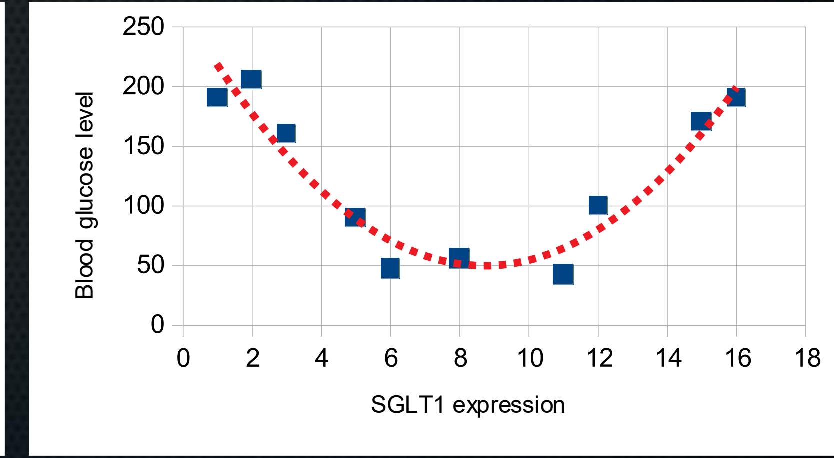

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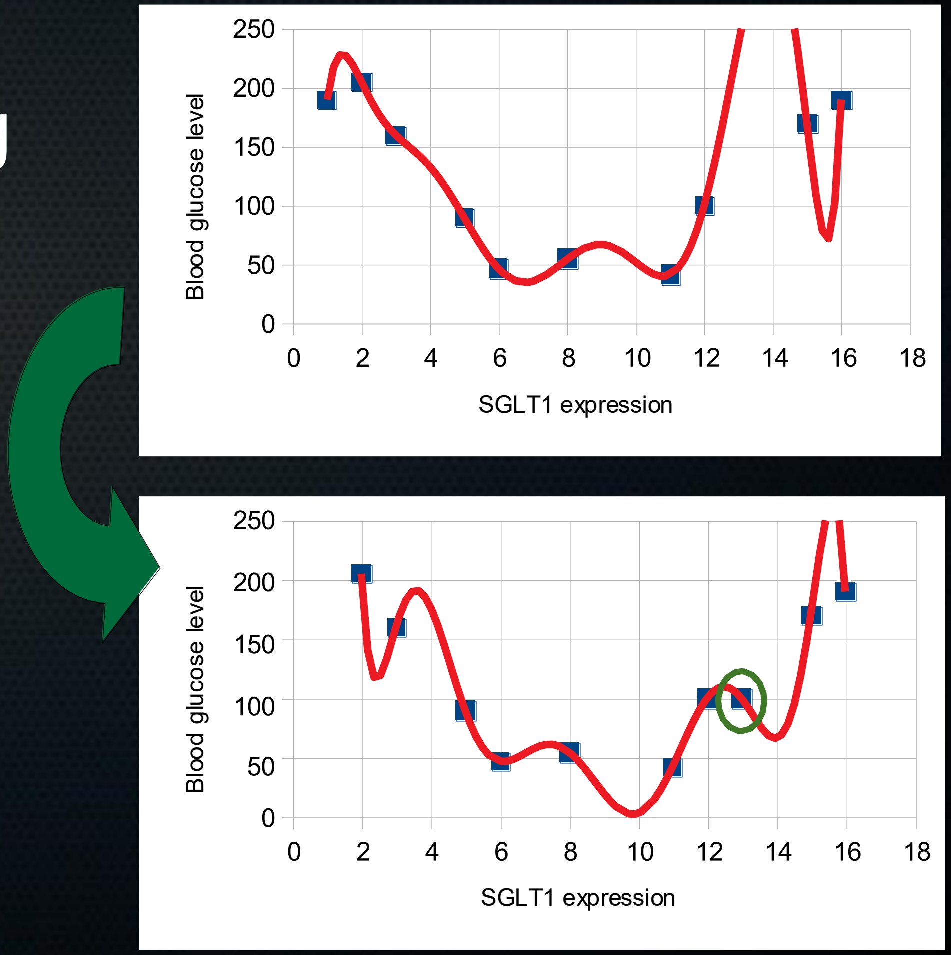
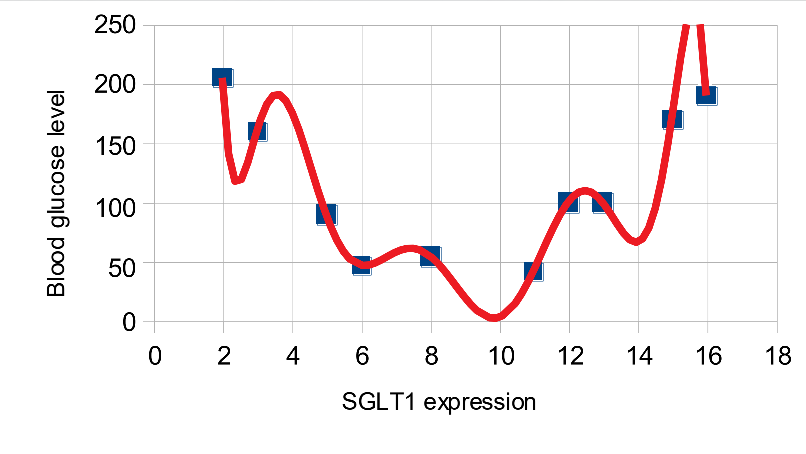
  -used x^1-x^9 as features
  -If we add one point:



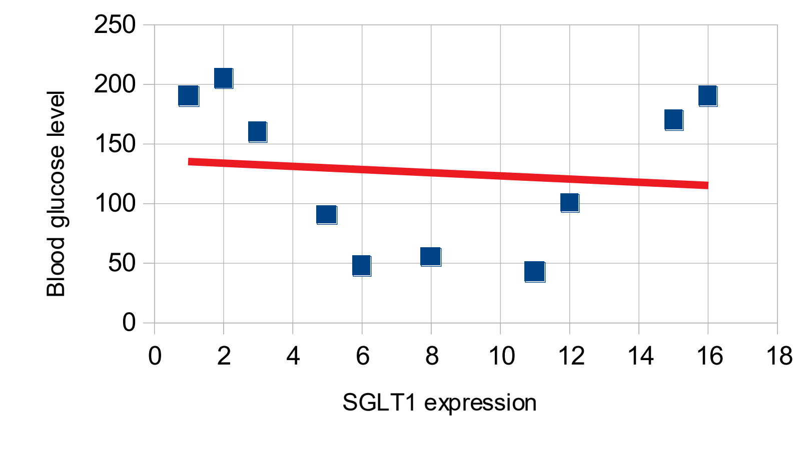
How to generalise well

- High **variance**:
  -Huge amount of possible functions that pass through all points: large hypothesis space, can basically fit all the training data we give perfectly!
  -Do great on this data, but will
  fare poorly when predicting unseen data



How to generalise well

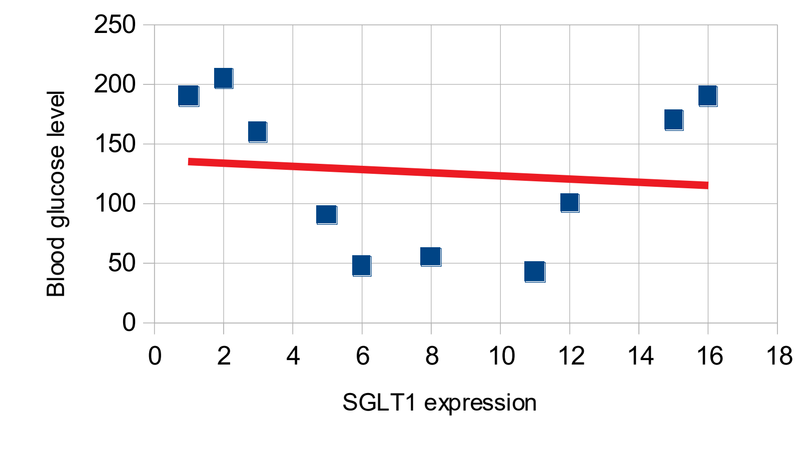
- High **bias**:
  -error introduced by approximating a complex process with a simple model.
  -Only 1 feature (intercept + theta1)



How to generalise well

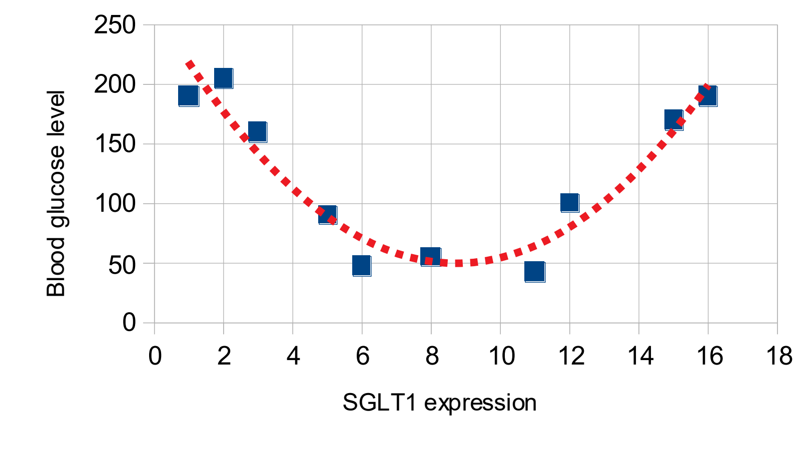
- High **bias**:

  -error introduced by approximating a complex process with a simple model.
  -Only 1 feature (intercept + theta1)
  -Data clearly shows that a linear curve is not the best fit, yet we keep our preconception, or *bias*, that it should adhere to a univariate linear regression
  -Does poorly on this data and will also fare poorly when predicting unseen data

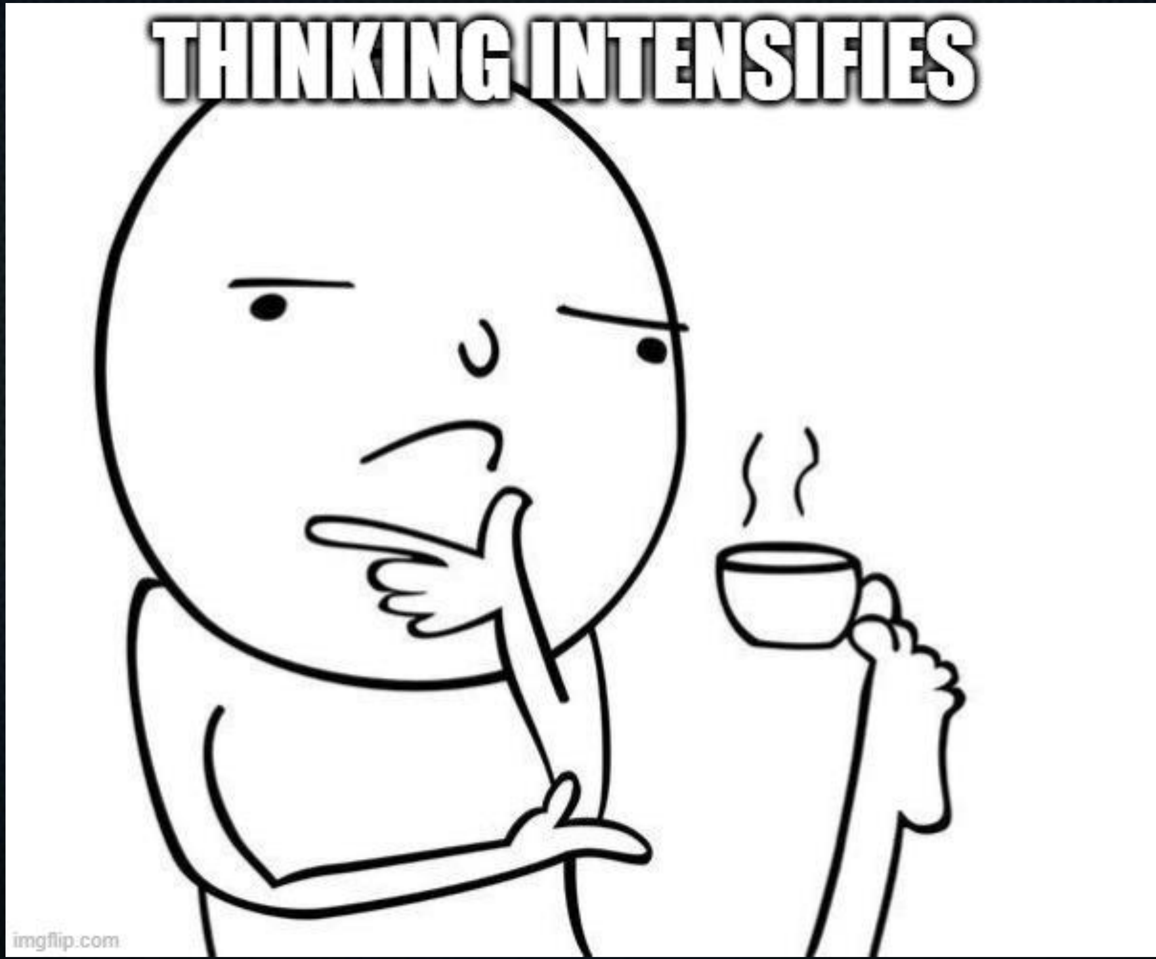


How to generalise well

- Just right:
  -Not fit too closely to known examples, probably generalises well.



What can we do to find a good model?



What can we do to find a good model?

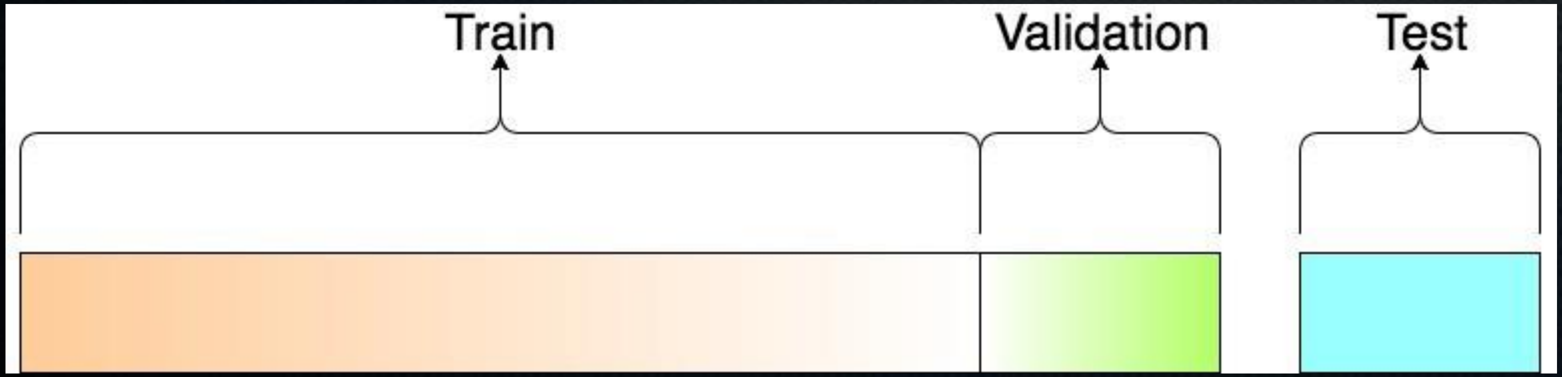
- Find a way to approximate generalisation error: how well do you do on unseen data?
- See how error on seen and unseen data changes with amount of training data (plot learning curves)
- ~~Reduce dimensionality by using only certain features~~
- Automatically constrain the fitting by penalising the cost function for too many/too large parameters

What can we do to find a good model?

- ***Find a way to approximate generalisation error: how well do you do on unseen data?***
- See how error on seen and unseen data changes with amount of training data (plot learning curves)
- Automatically constrain the fitting by penalising the cost function for too many/too large parameters

Approximate generalisation error: split data

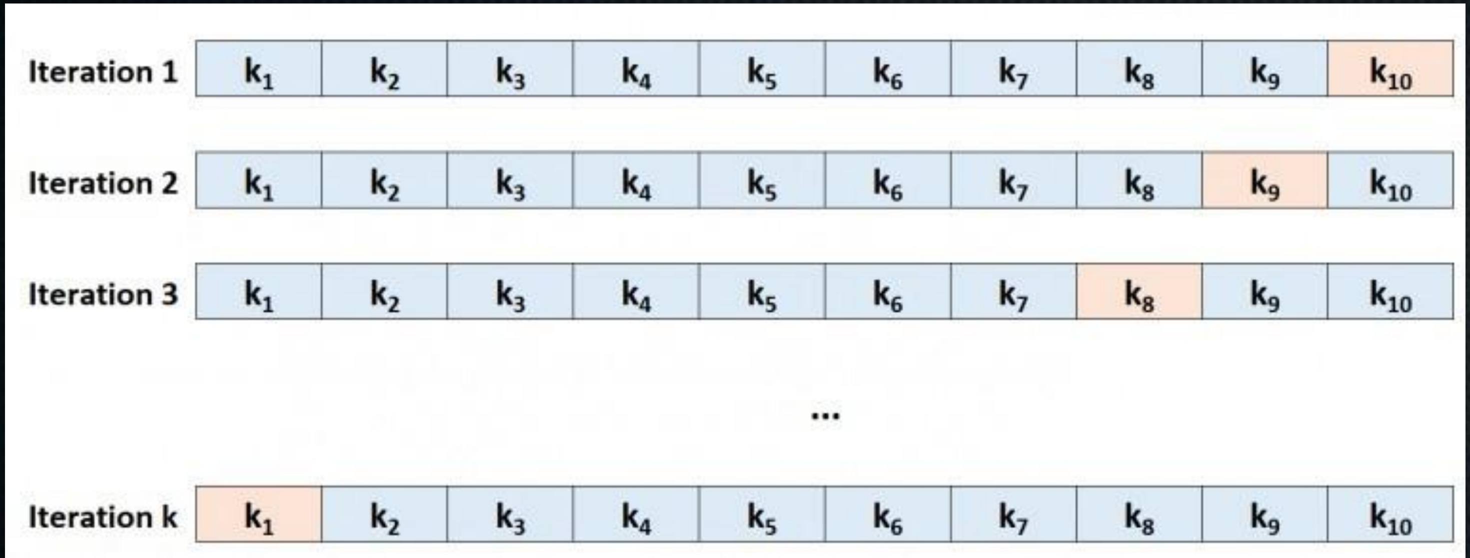
- Split data into training data, validation data, and a test set
- Test set: completely untouched until you are done training
- Train set: train your classifier on this
- Validation set: test your trained classifier on this



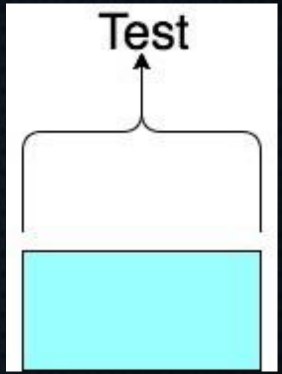
Source: https://stackoverflow.com/questions/56099495/what-should-be-passed-as-input-parameter-when-using-train-test-split-function-tw

Approximate generalisation error: split data

- K-fold cross-validation (often 10-fold):



Source:https://www.statology.org/k-fold-cross-validation/



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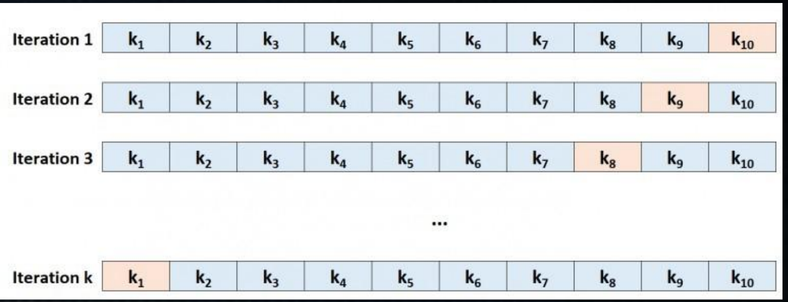
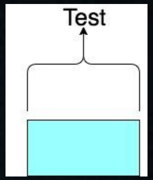
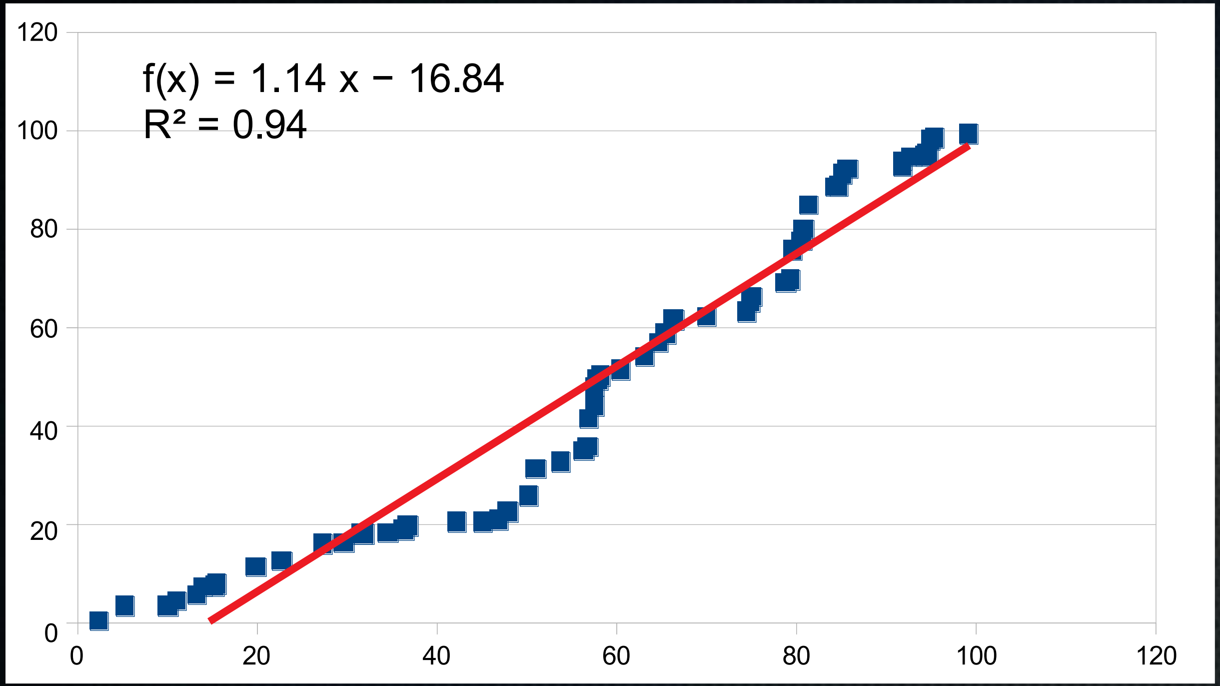




- Procedure:
  -Shuffle the data
  -Divide into k folds (e.g. 10 folds of 100 training examples each)
  - For each fold:
    -find parameters by minimising cost function on training set with gradient descent
    -predict on validation data
    -calculate cost on validation data (you know the true values)

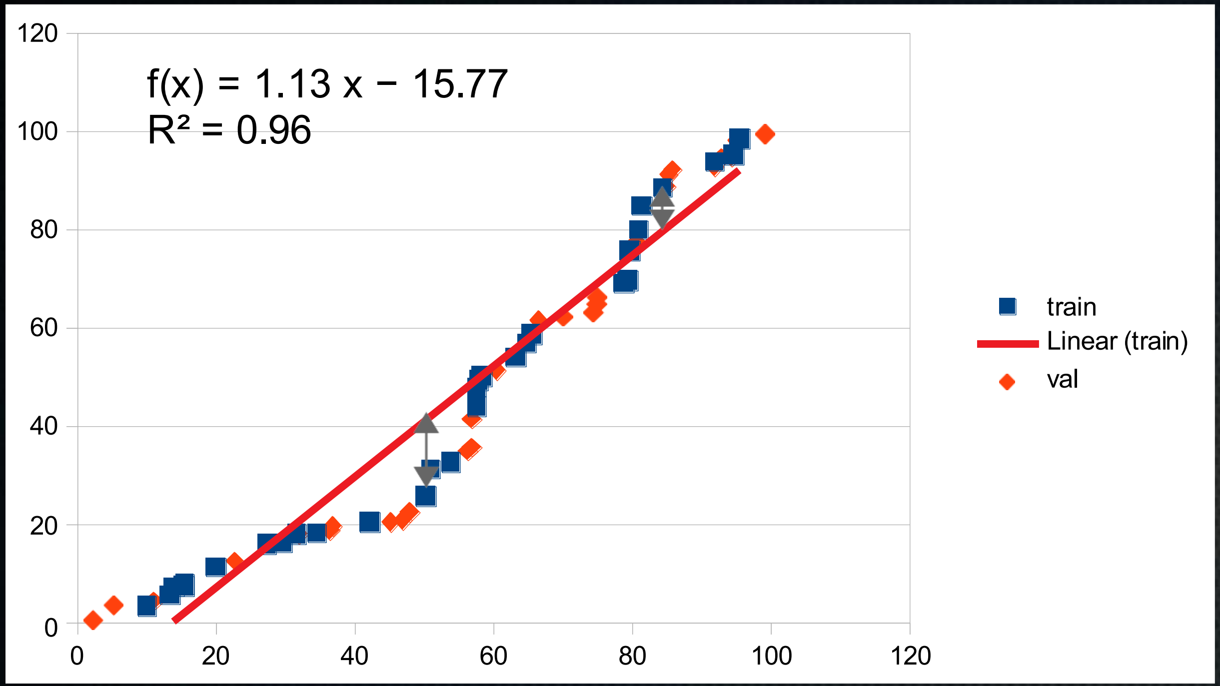
  -Average validation cost over folds ~ generalisation error

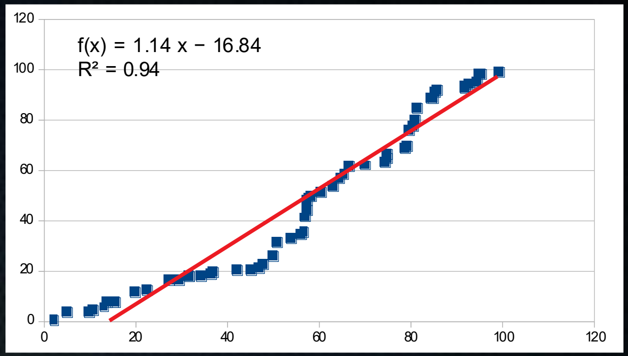
Example 2-fold cv on linear regression



All data

Example 2-fold cv on linear regression: fold 1





All data

$$J(\theta_0,\theta_1)_{train} = \frac{1}{2m_{train}} \sum_{i=1}^{m_{train}} (h_\theta(x^{(i)}) - y^{(i)})^2 = 41{,}66$$

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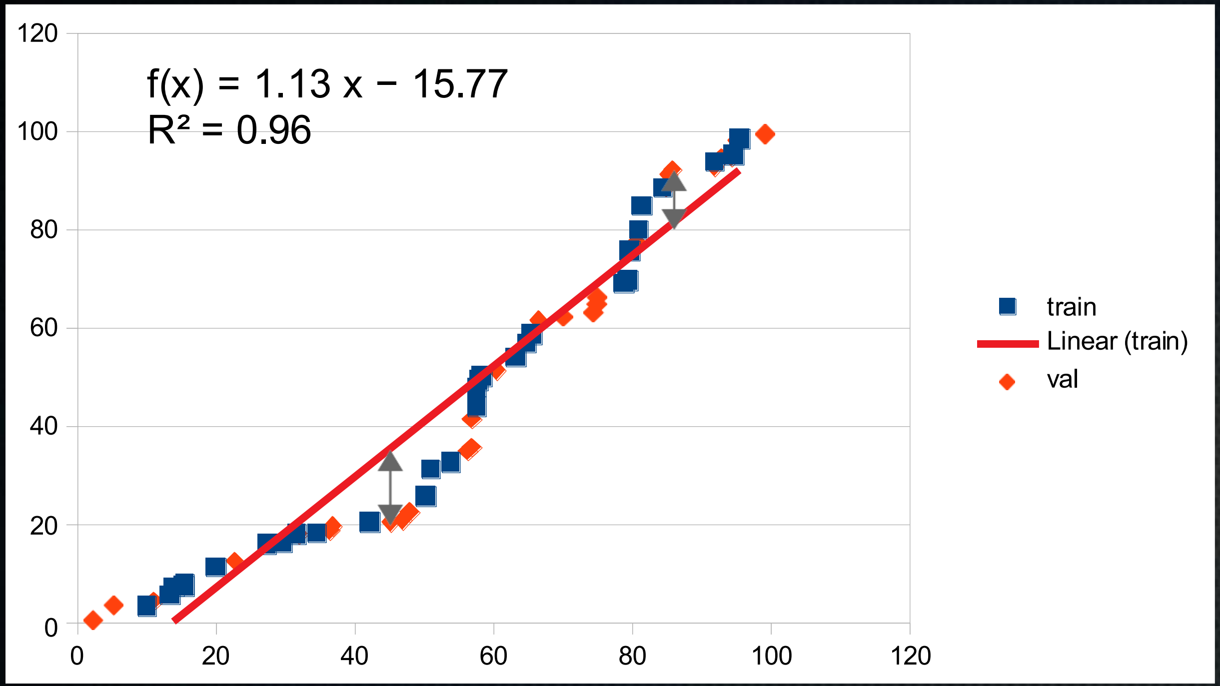
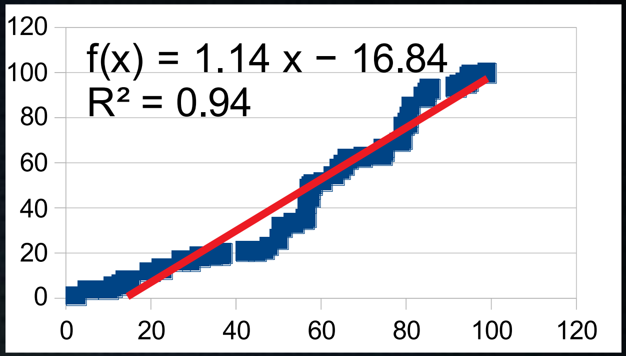


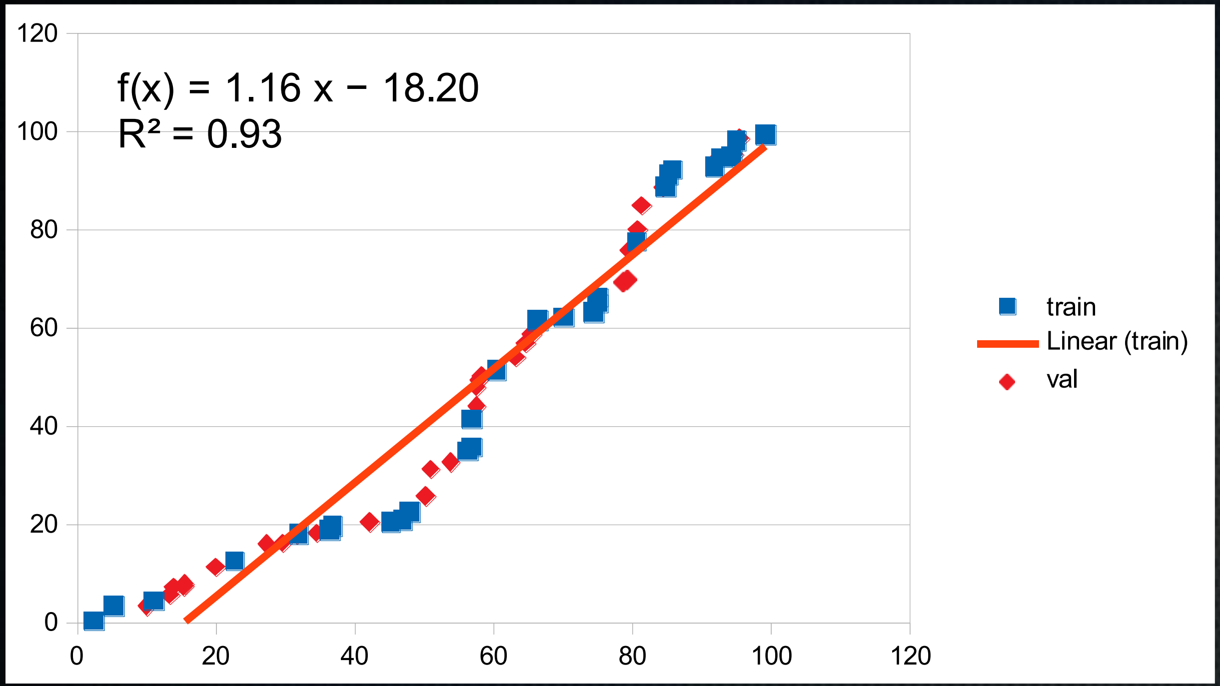


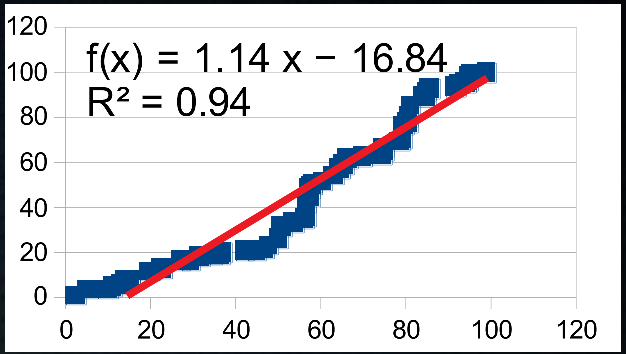
All data

$$J(\theta_0,\theta_1)_{train}=\frac{1}{2m_{train}}\sum_{i=1}^{m_{train}}(h_\theta(x^{(i)})-y^{(i)})^2=41,66$$

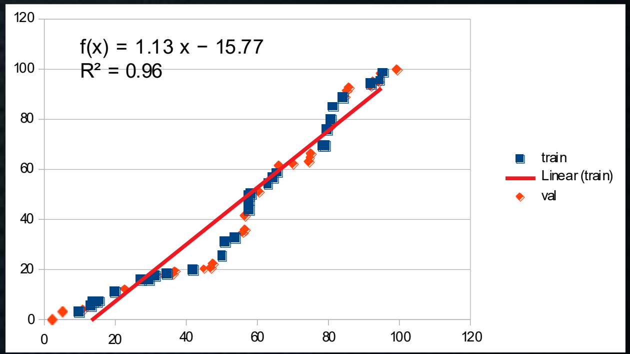
$$J(\theta_0,\theta_1)_{val}=\frac{1}{2m_{val}}\sum_{i=1}^{m_{val}}(h_\theta(x^{(i)})-y^{(i)})^2=52,34$$

Example 2-fold cv on linear regression: fold 2





All data



$$J(\theta_0,\theta_1)_{train} = \frac{1}{2m_{train}}\sum_{i=1}^{m_{train}} (h_\theta(x^{(i)}) - y^{(i)})^2 = 75{,}25$$

$$J(\theta_0,\theta_1)_{val} = \frac{1}{2m_{val}}\sum_{i=1}^{m_{val}} (h_\theta(x^{(i)}) - y^{(i)})^2 = 43$$

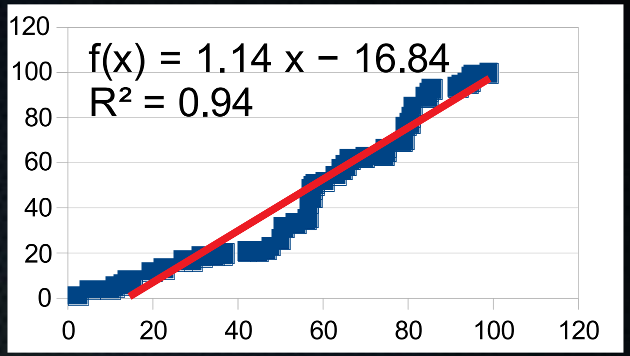
$$J(\theta_0,\theta_1)_{train} = 41{,}66$$

$$J(\theta_0,\theta_1)_{val} = 52{,}34$$

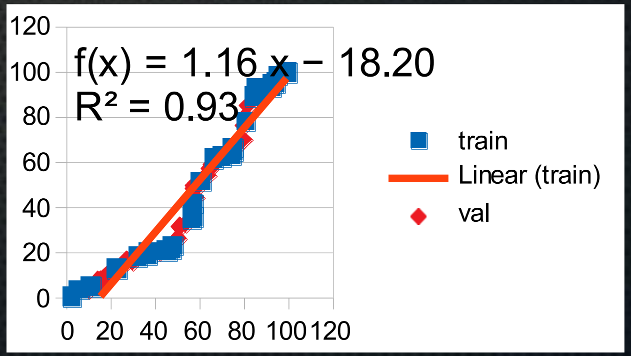
Fold 1

Example 2-fold cv on linear regression

- Avg. train error: 58,5
- Avg. Validation error: 47,7
- Finally: would train on all data and test that on test set.

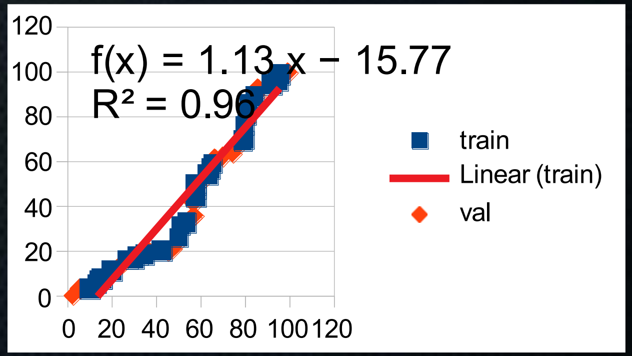


All data



$$J(\theta_0,\theta_1)_{train}=75,25$$
$$J(\theta_0,\theta_1)_{val}=43$$

Fold 2



$$J(\theta_0,\theta_1)_{train}=41,66$$
$$J(\theta_0,\theta_1)_{val}=52,34$$

Fold 1

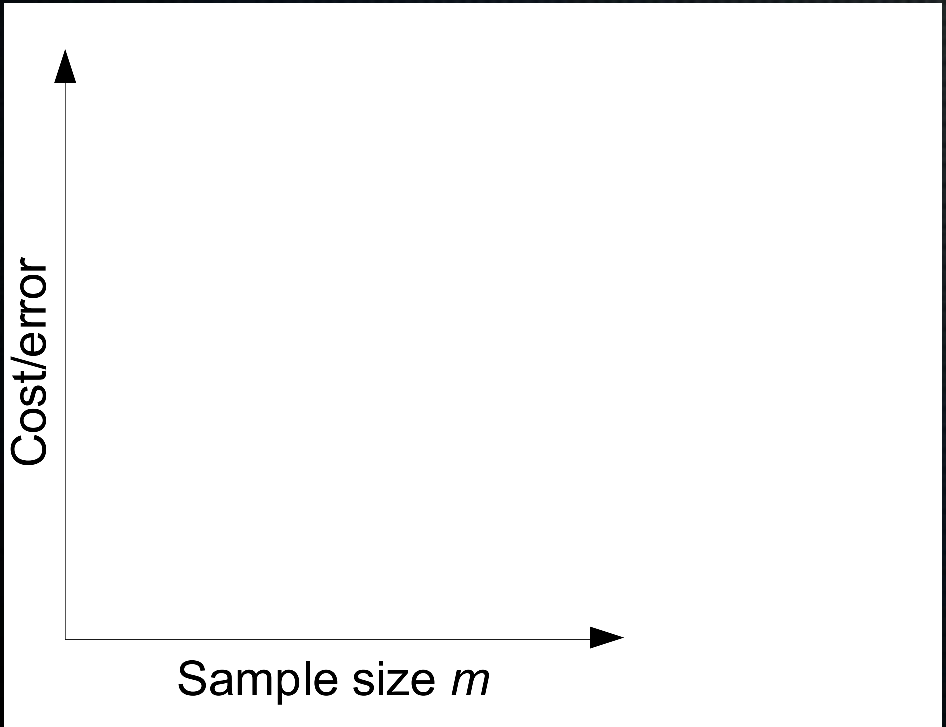
What can we do to find a good model?

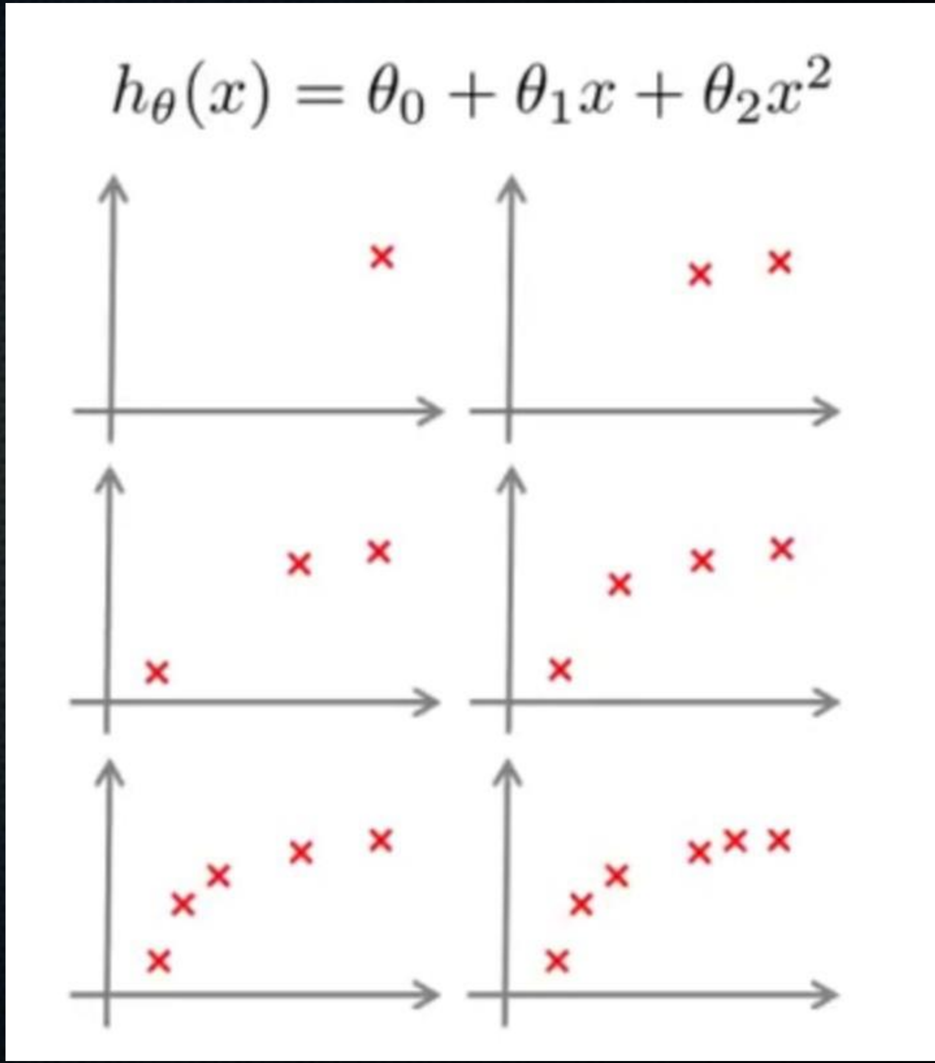
- ~~Find a way to approximate generalisation error: how well do you do on unseen data?~~
- ***<u>See how error on seen and unseen data changes with amount of training data (plot learning curves)</u>***
- Automatically constrain the fitting by penalising the cost function for too many/too large parameters

Learning curves

$$J_{train} = \frac{1}{2m_{train}} \sum_{i=1}^{m_{train}} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$$J_{val} = \frac{1}{2m_{val}} \sum_{i=1}^{m_{val}} (h_\theta(x^{(i)}) - y^{(i)})^2$$





Source: Andrew Ng, Coursera

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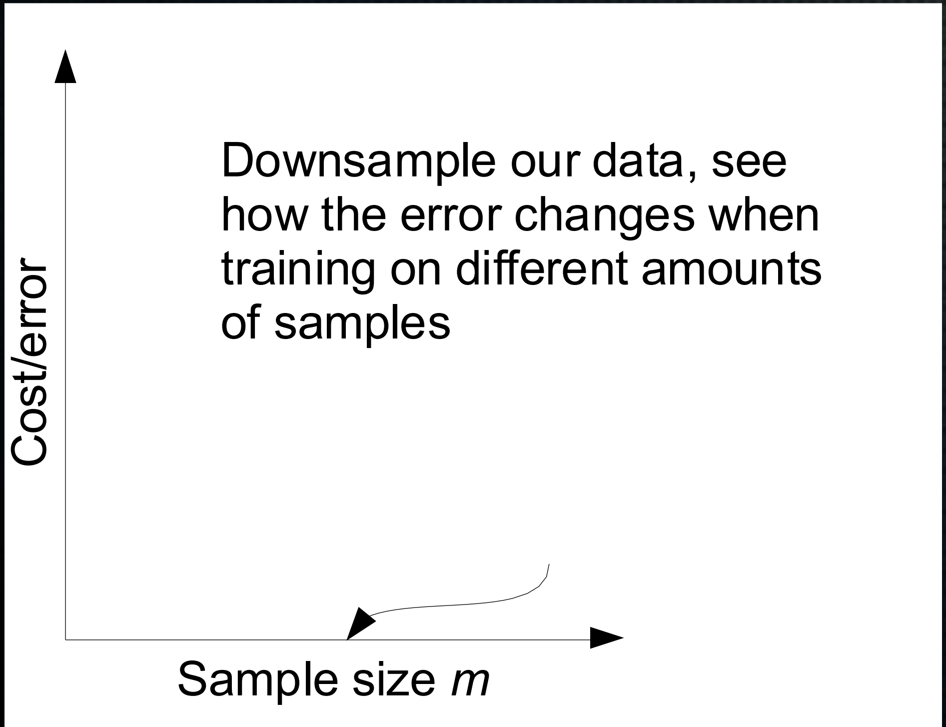

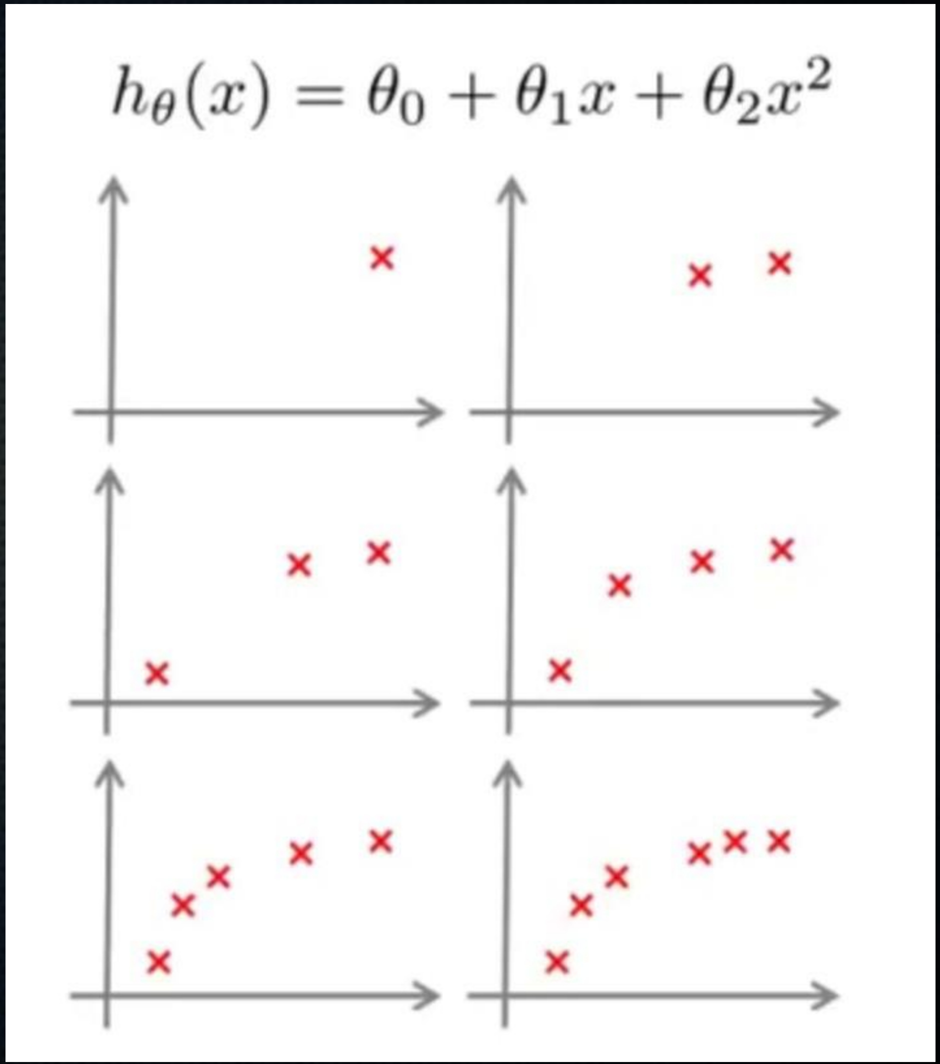

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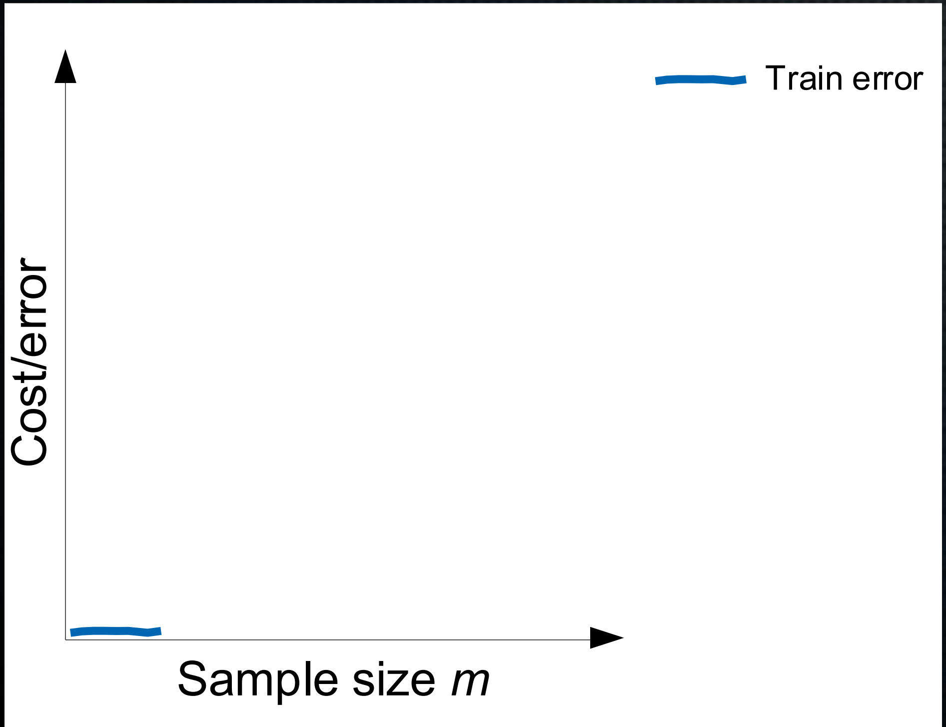
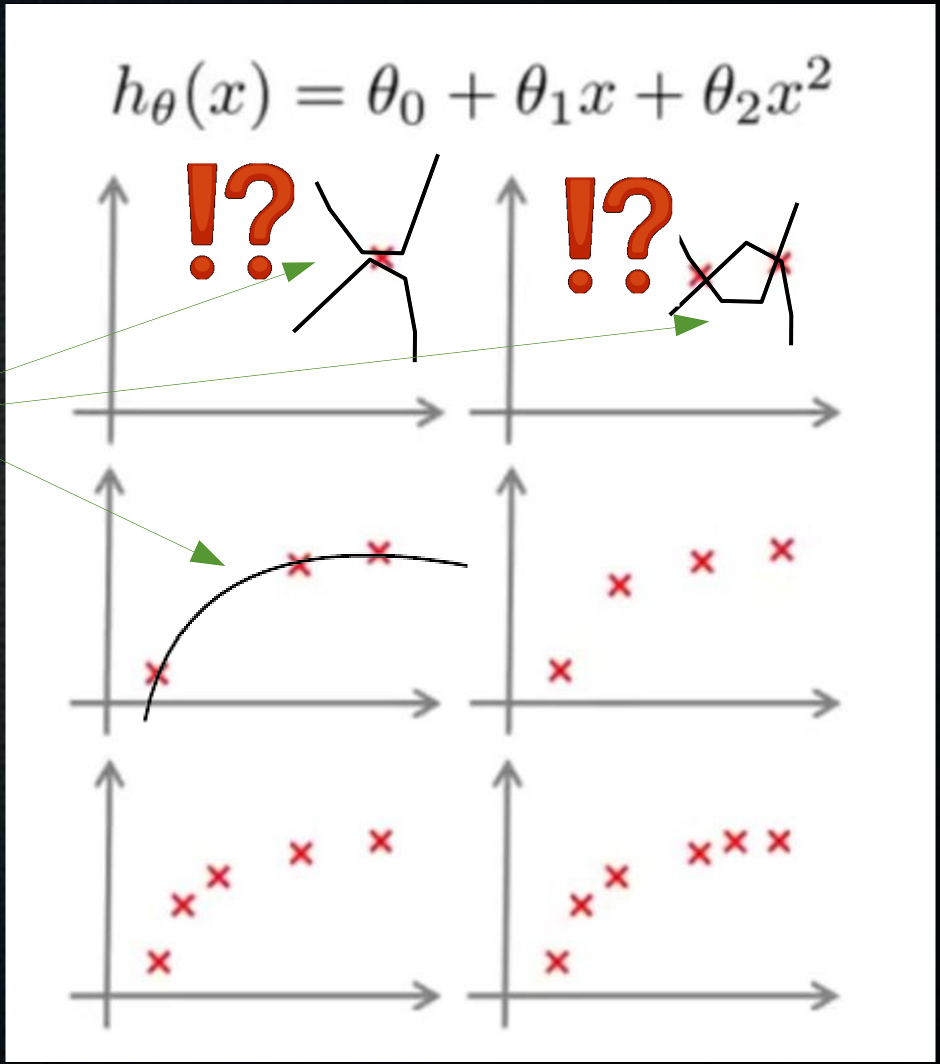


Easy to fit few datapoints perfectly



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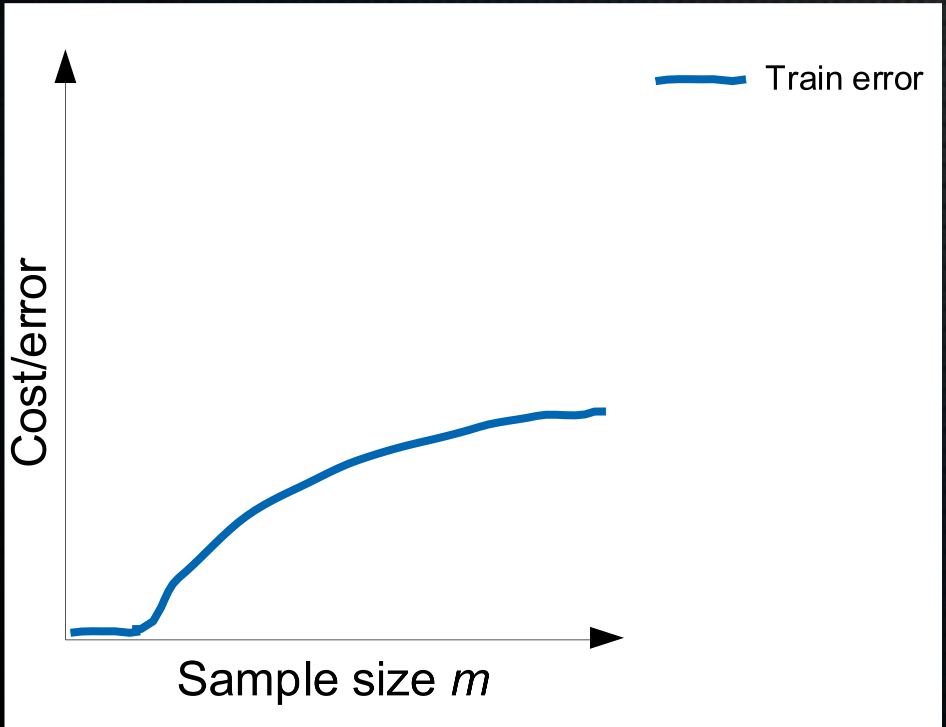
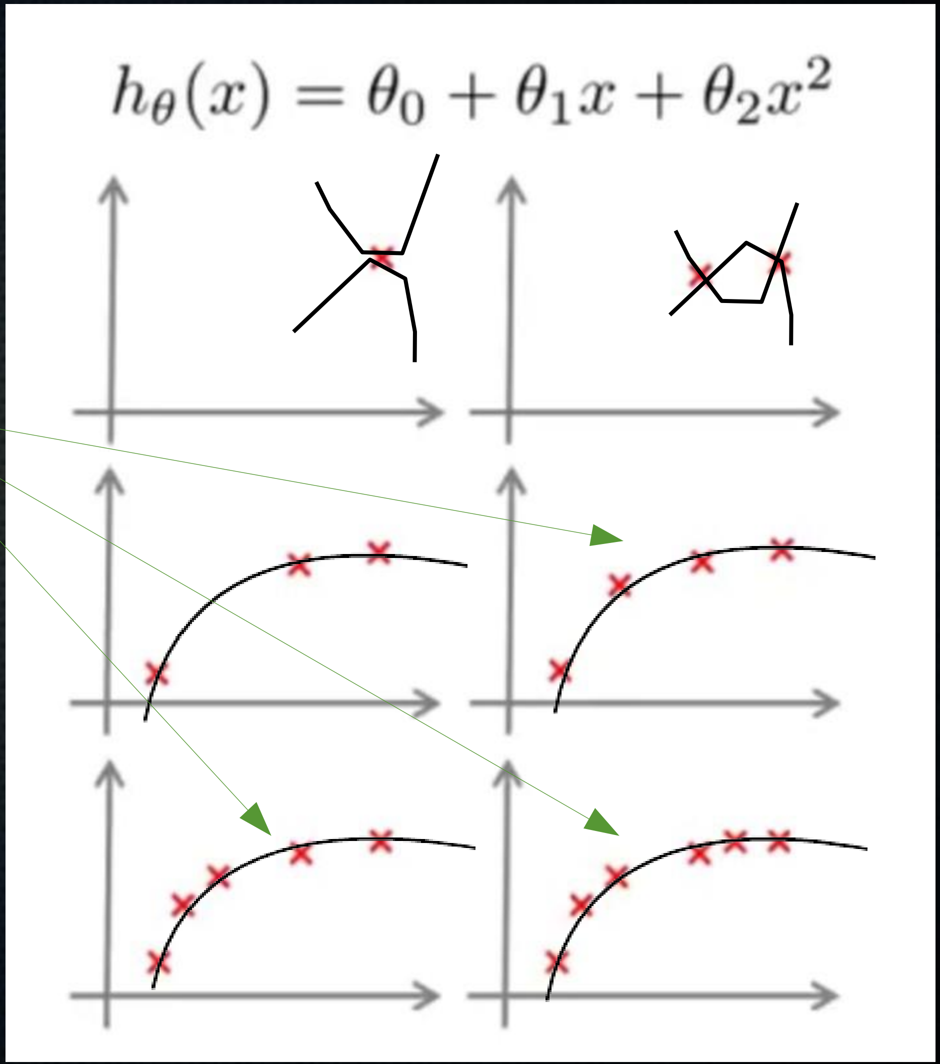


Harder and harder to fit everything perfectly



Source: Andrew Ng, Coursera

Learning curves

$$J_{train} = \frac{1}{2m_{train}} \sum_{i=1}^{m_{train}} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

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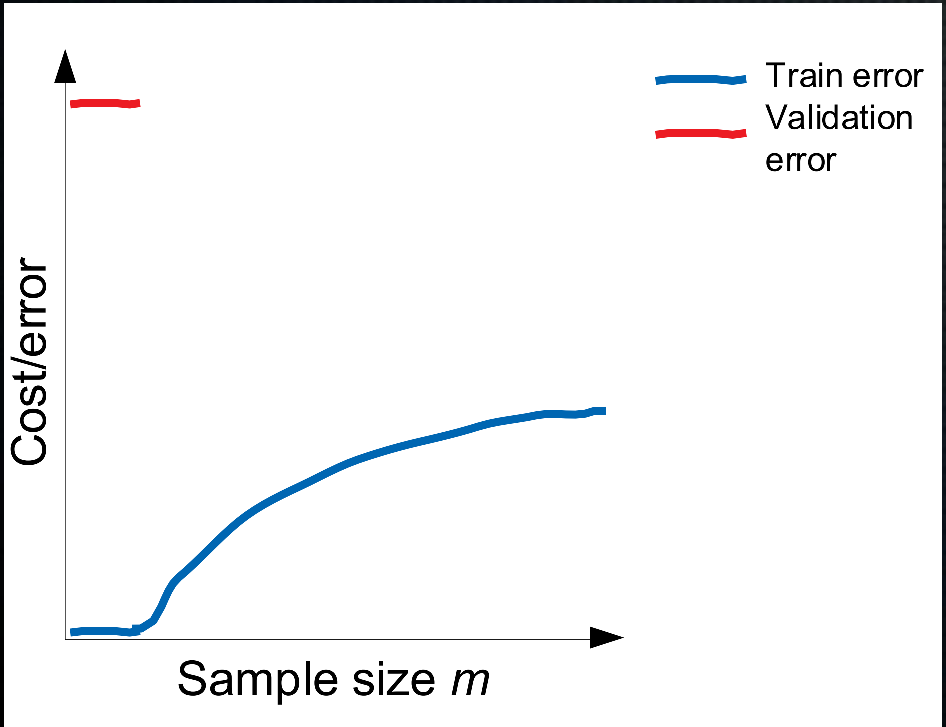
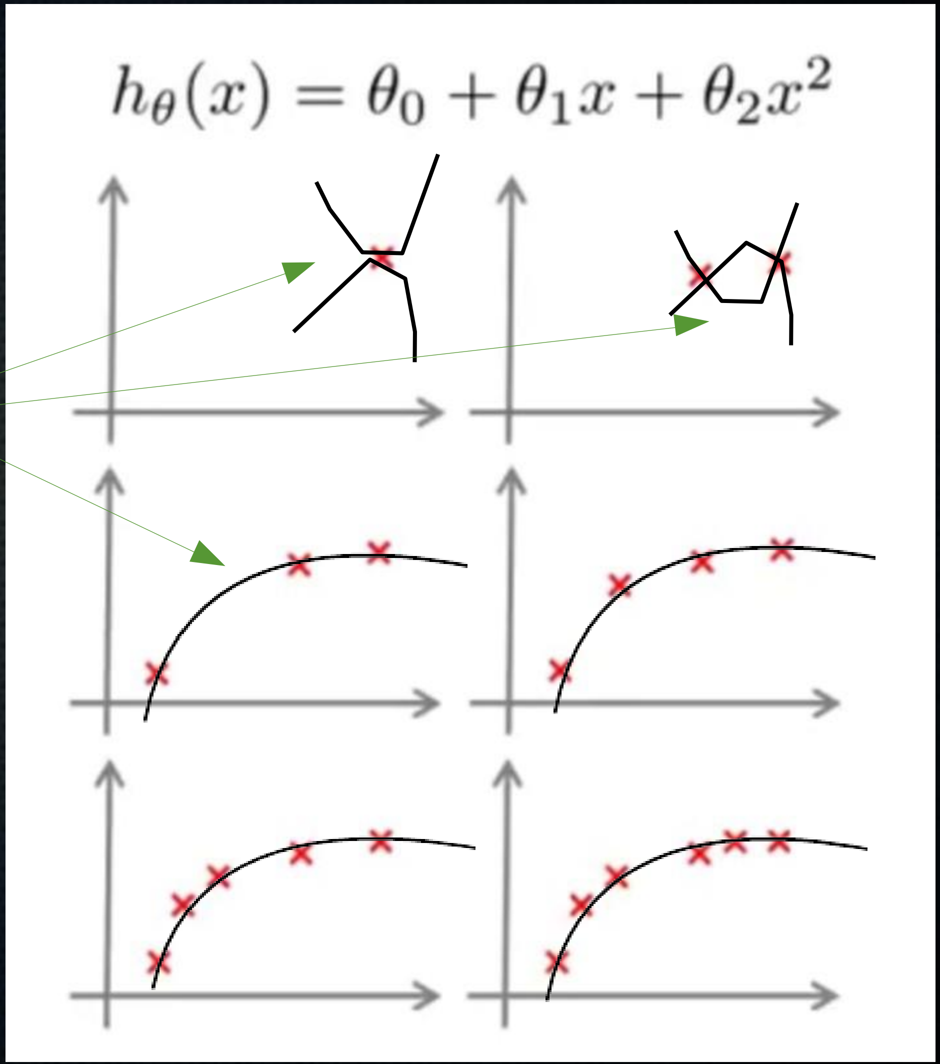


Generalises poorly to new data



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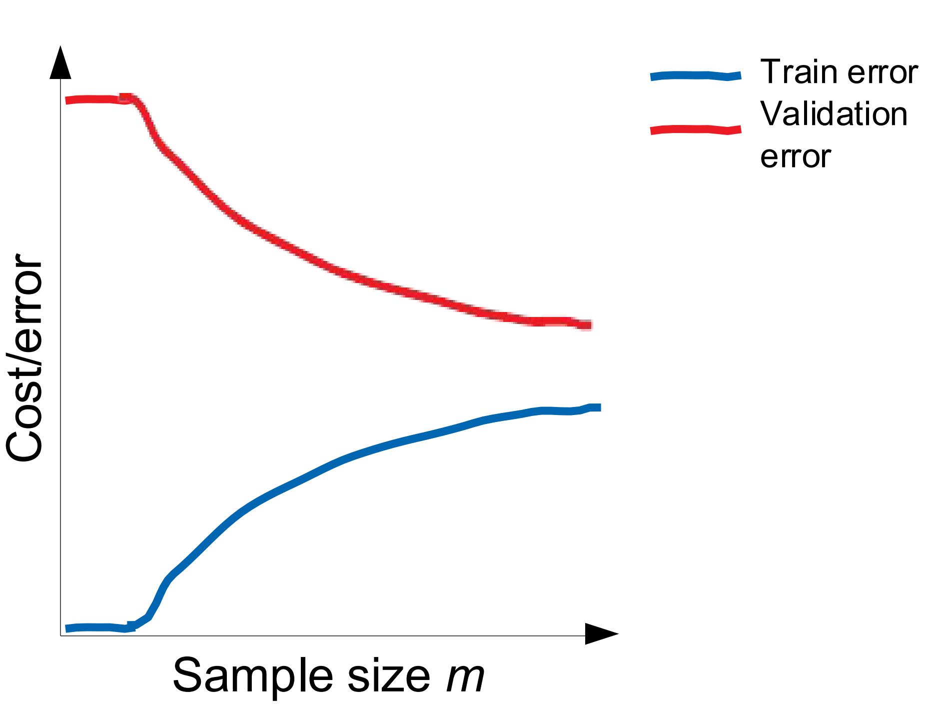
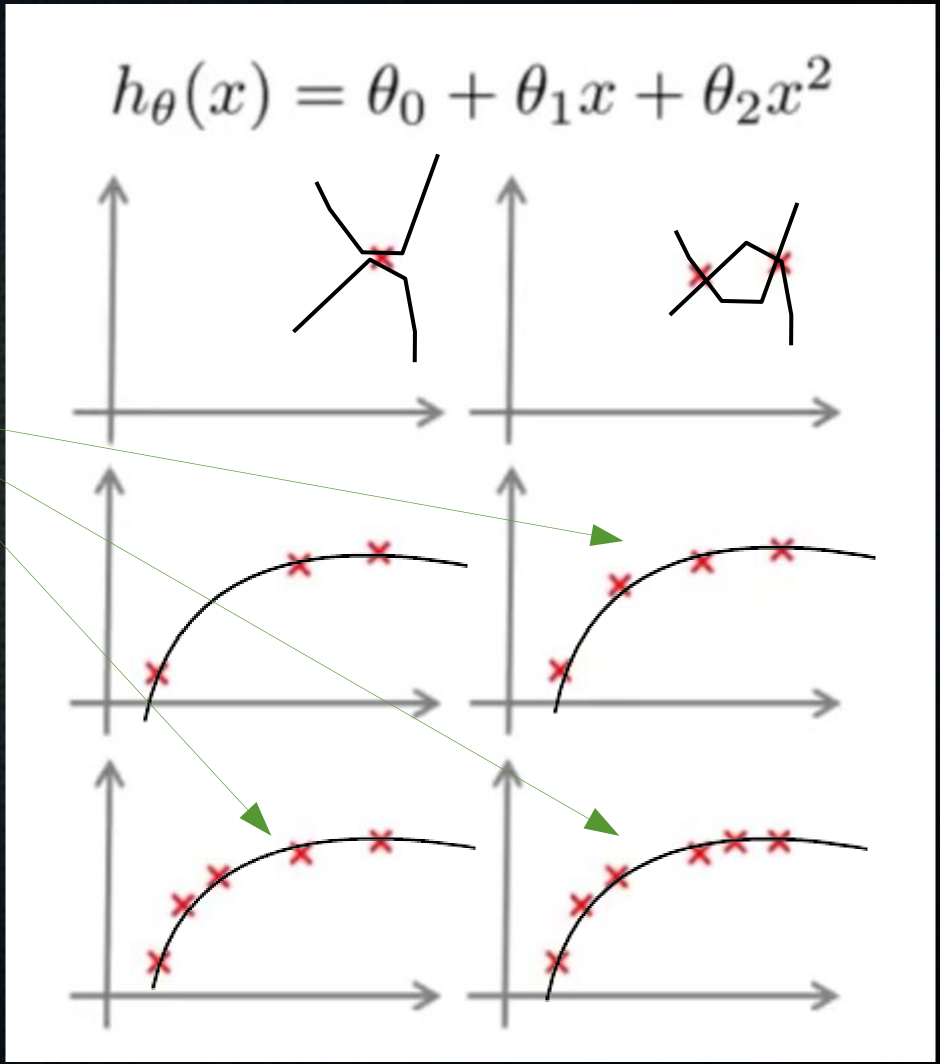


Generalises better to new data



Source: Andrew Ng, Coursera

Learning curves: high bias

$$J_{train} = \frac{1}{2m_{train}} \sum_{i=1}^{m_{train}} (h_\theta(x^{(i)}) - y^{(i)})^2$$

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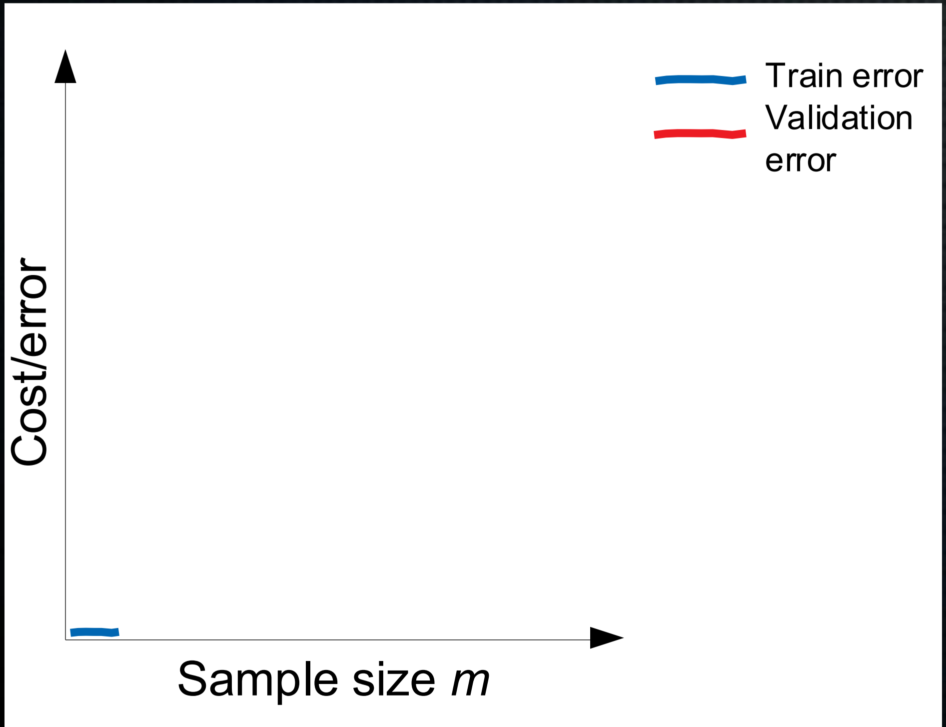
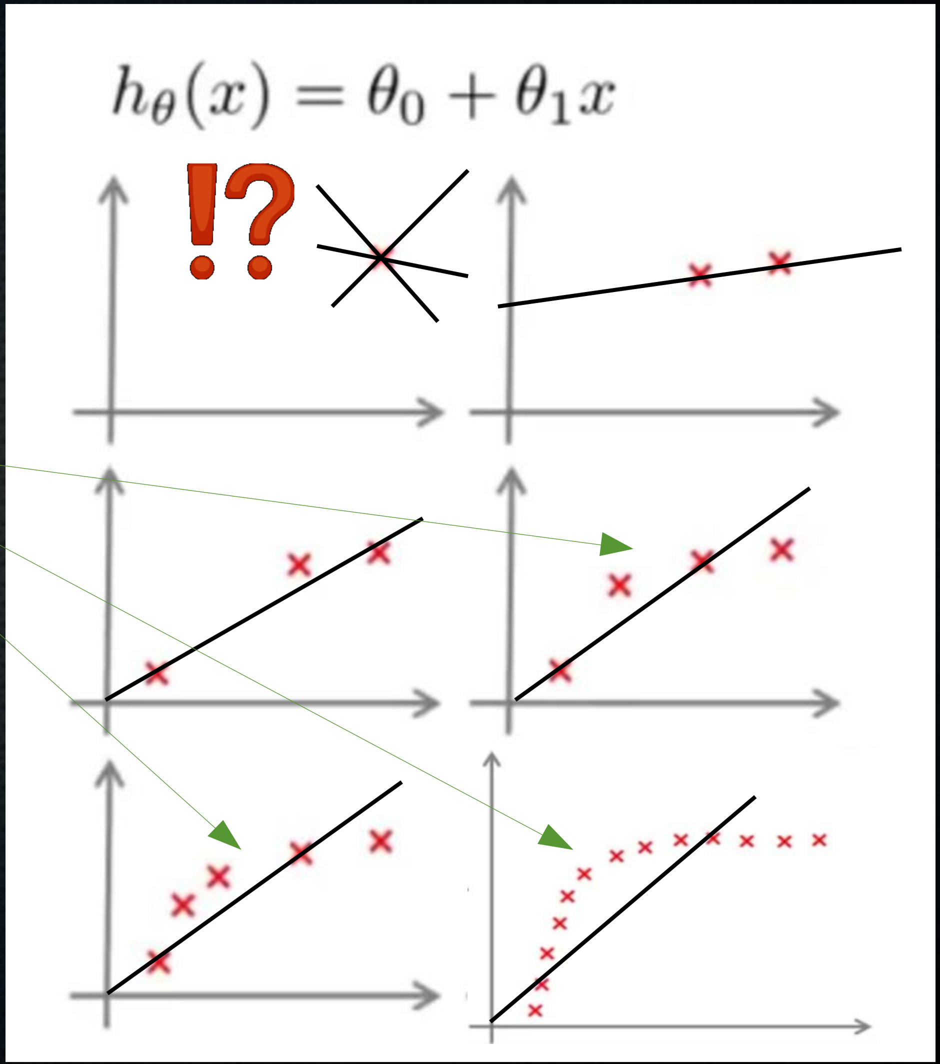


Keep pretty much the same line even as data increases



Source: Andrew Ng, Coursera

Learning curves: high bias

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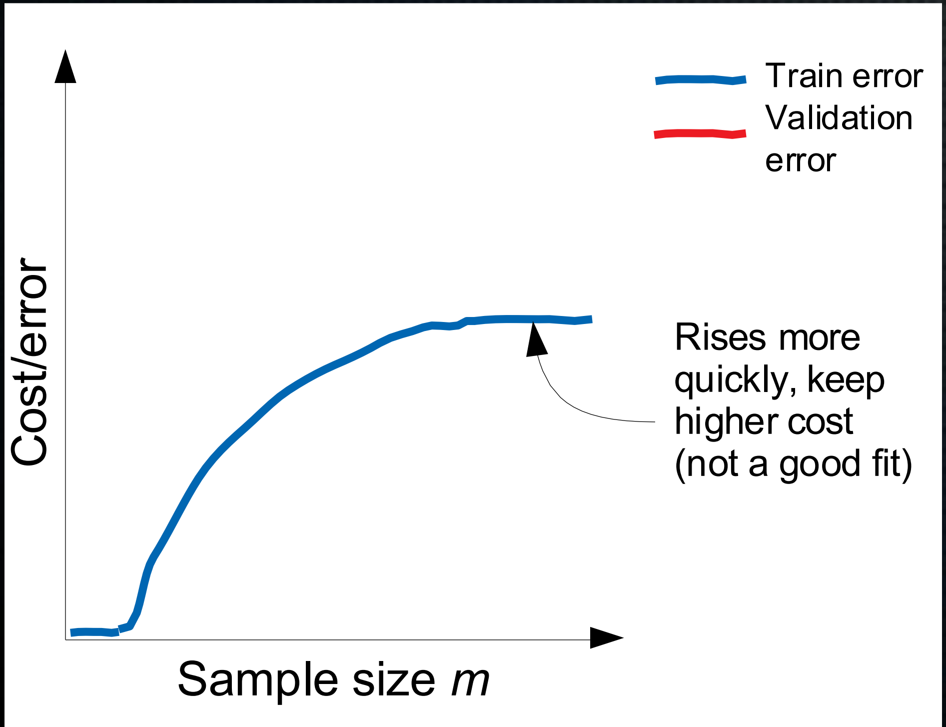

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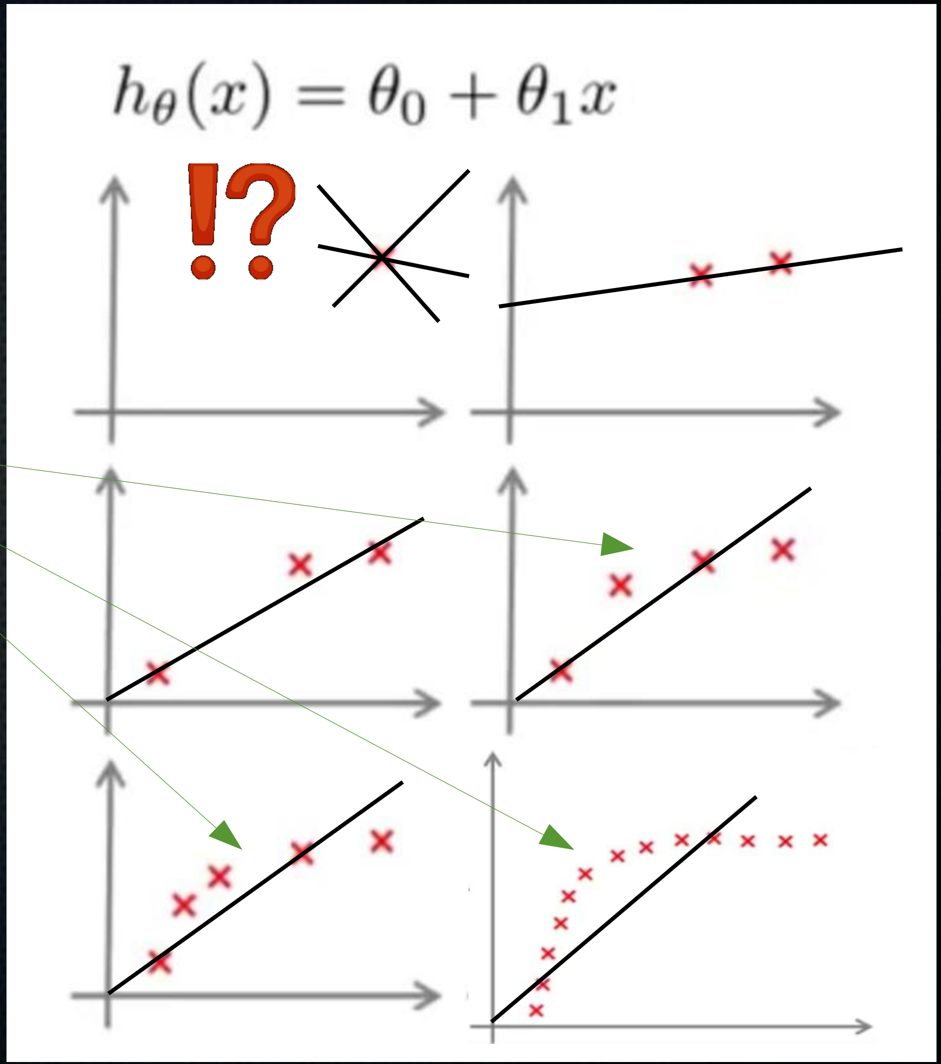

Source: Andrew Ng, Coursera

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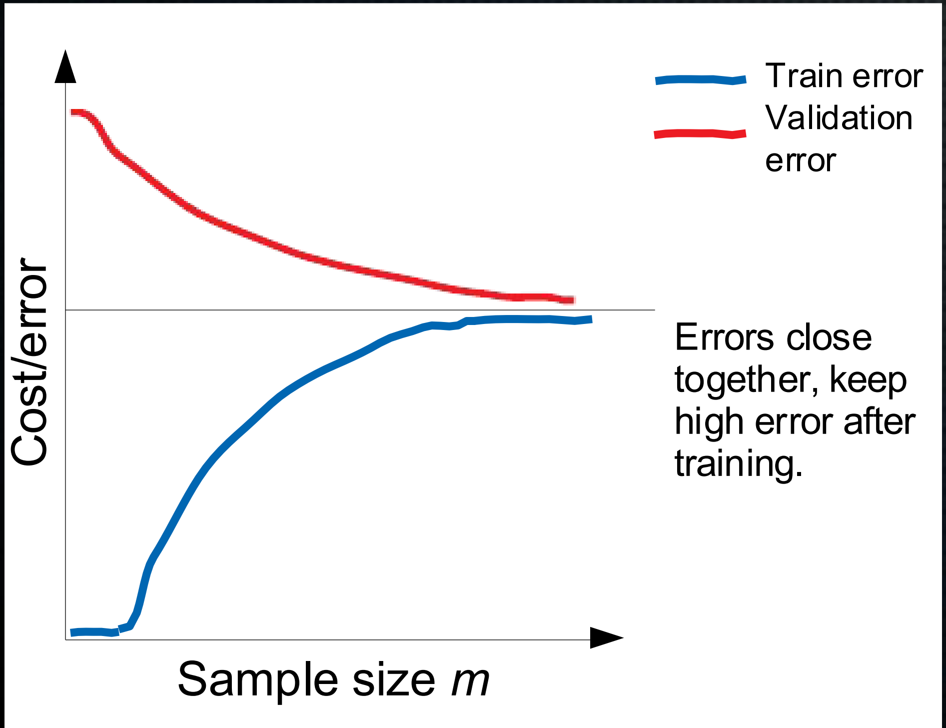

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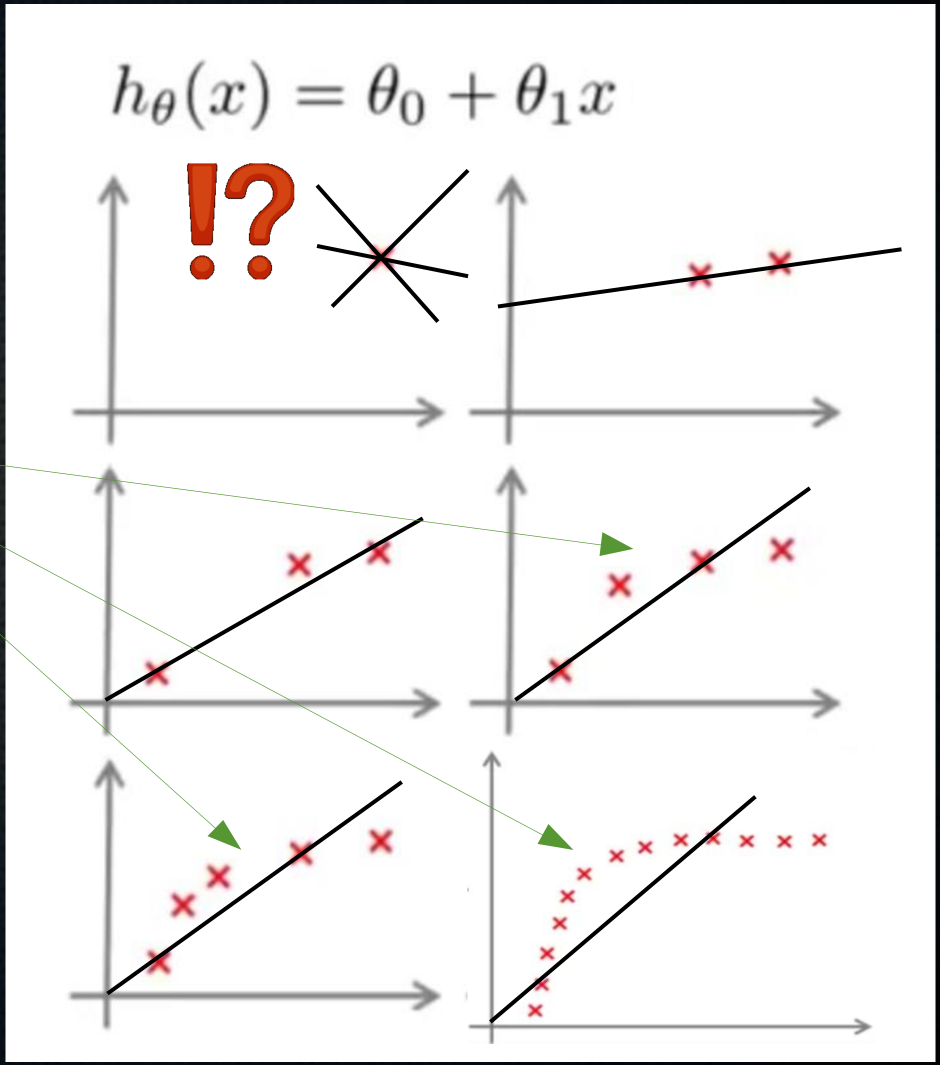


Source: Andrew Ng, Coursera

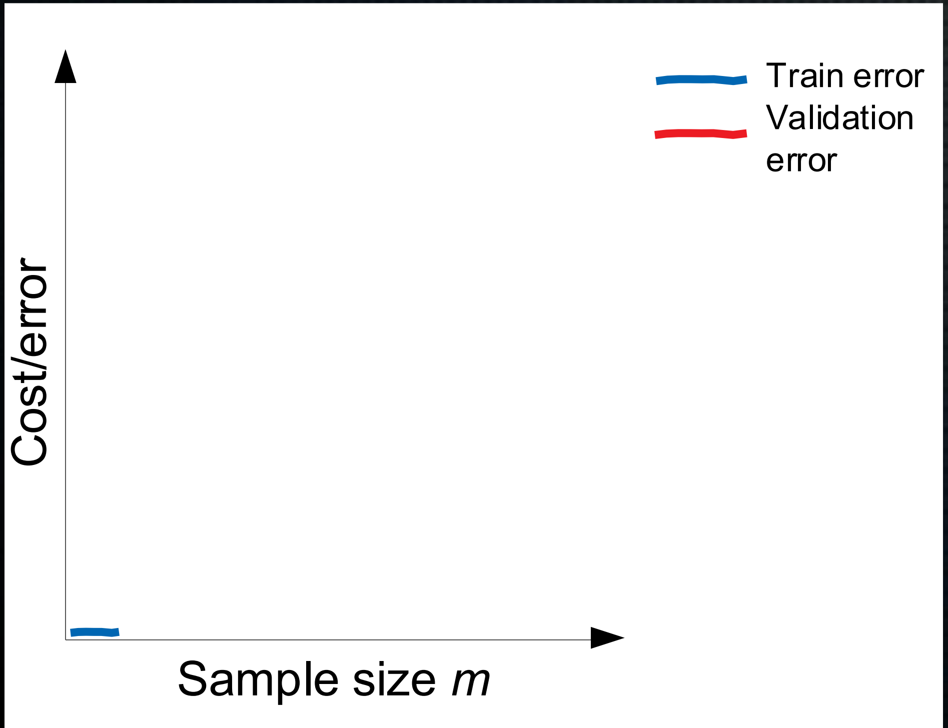
Learning curves: high bias

- If your learning algorithm is biased, getting more training data will not help!

Learning curves: high variance

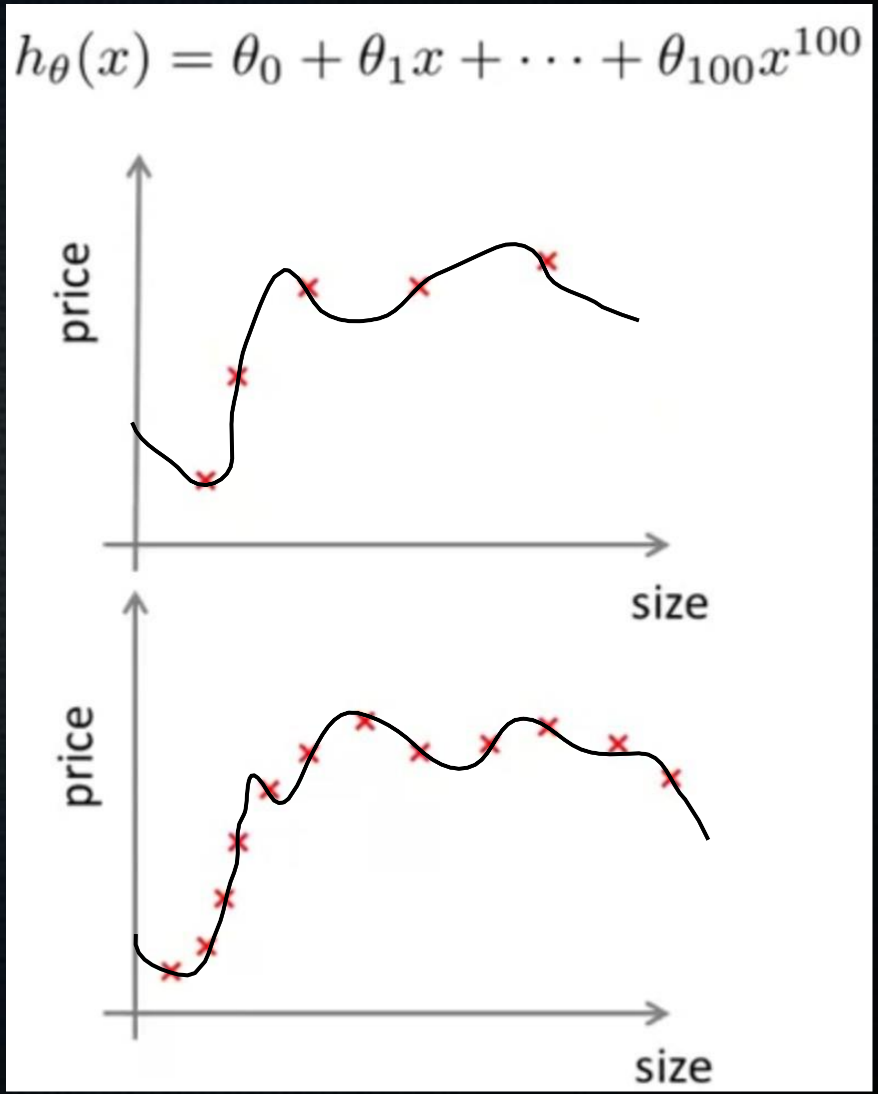
$$J_{train} = \frac{1}{2m_{train}} \sum_{i=1}^{m_{train}} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

$$J_{val} = \frac{1}{2m_{val}} \sum_{i=1}^{m_{val}} \left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$



Fit perfectly

Fit very well, but not perfect

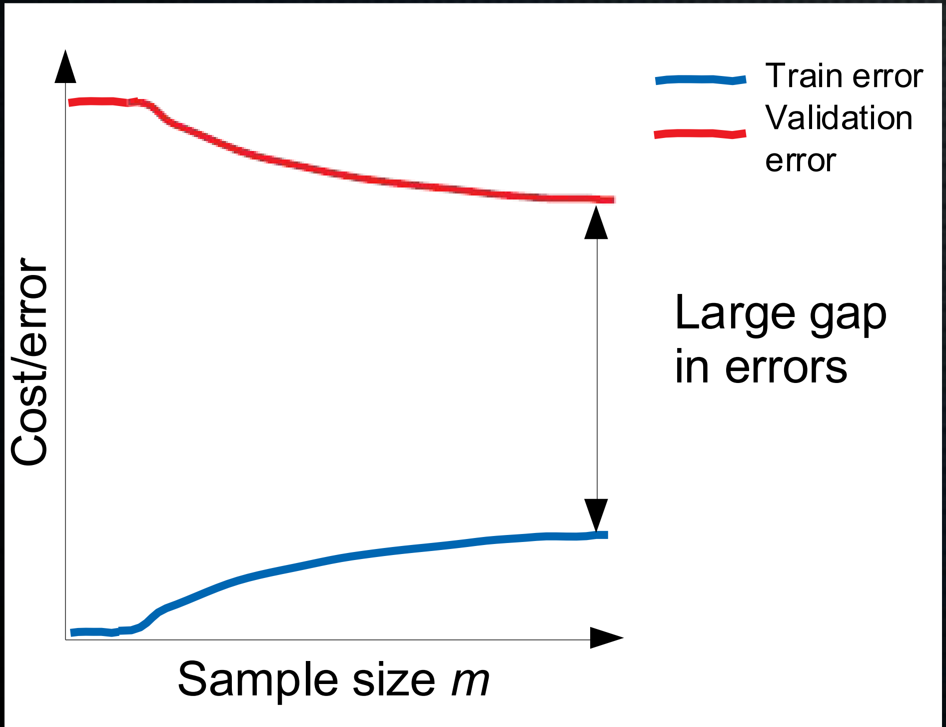


Source: Andrew Ng, Coursera

Learning curves: high variance

$$J_{train} = \frac{1}{2m_{train}} \sum_{i=1}^{m_{train}} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$$J_{val} = \frac{1}{2m_{val}} \sum_{i=1}^{m_{val}} (h_\theta(x^{(i)}) - y^{(i)})^2$$



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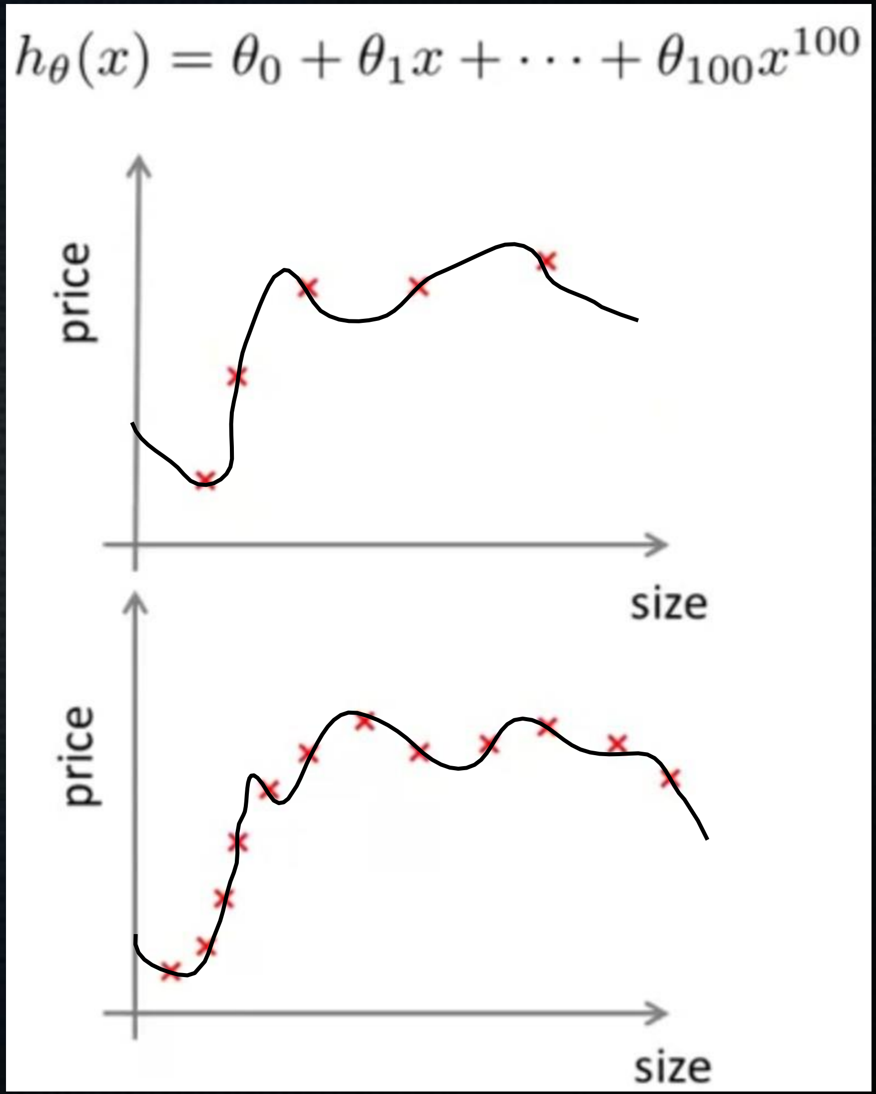

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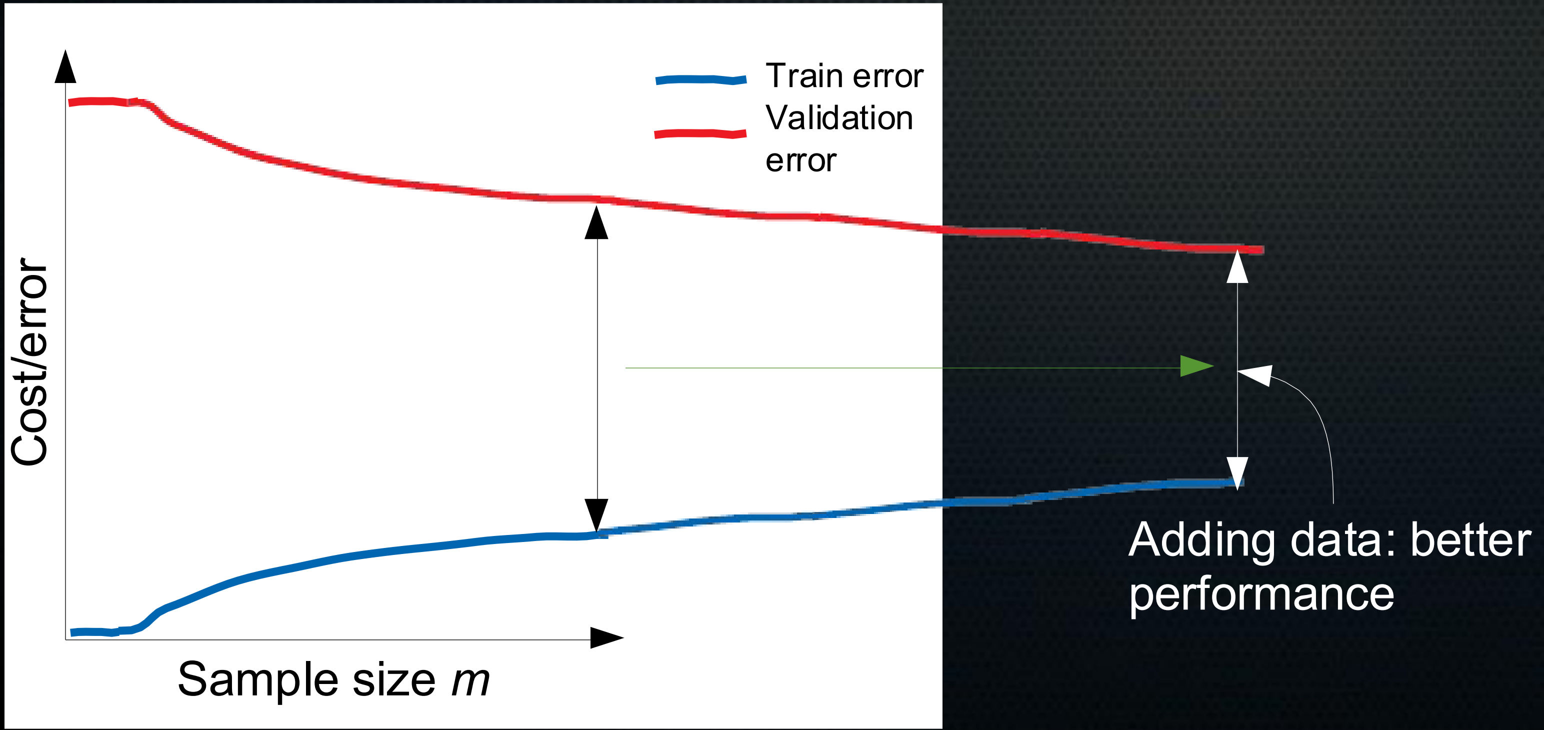
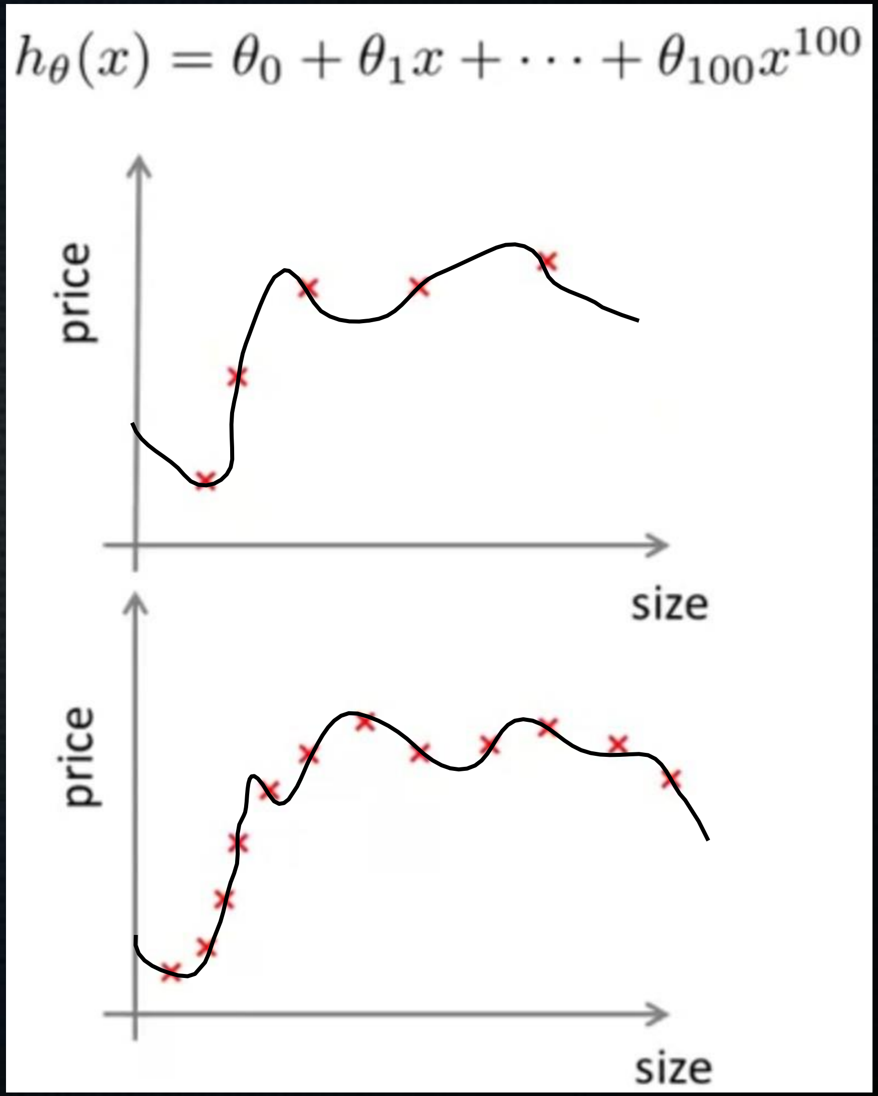
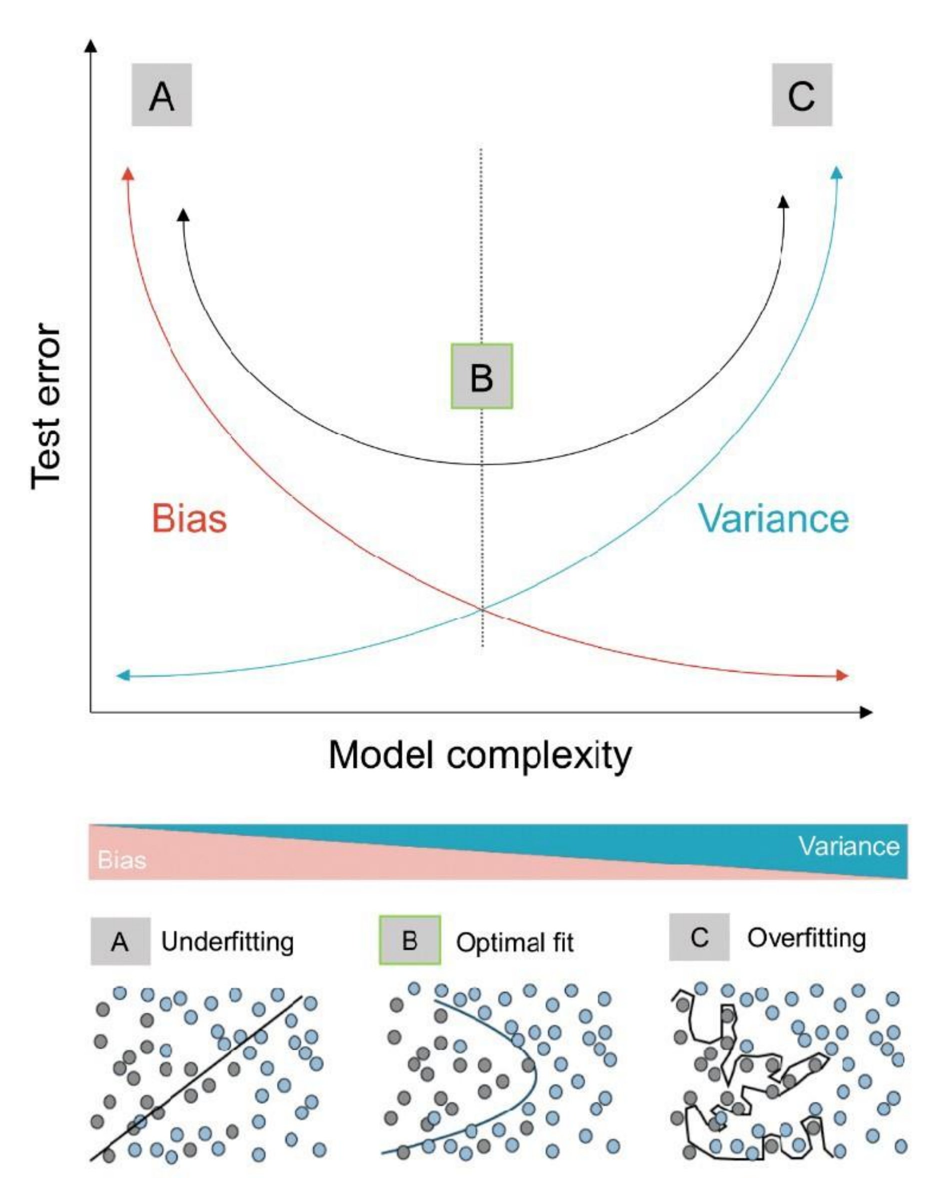




Source: Andrew Ng, Coursera

Learning curves

- There‘s a trade-off between bias and variance
- Learning curves allow you to diagnose what your algorithm might be suffering from



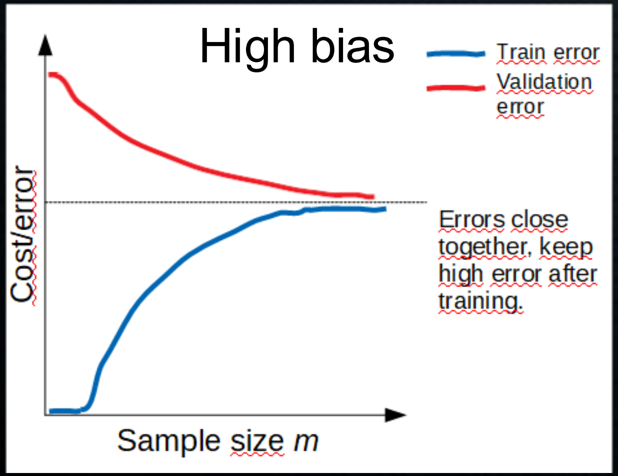
Source: Kernbach, J. M., & Staartjes, V. E. (2020). Machine learning-based clinical prediction modeling--A practical guide for clinicians. arXiv preprint arXiv:2006.15069.

Summary: cross-validation and learning curves

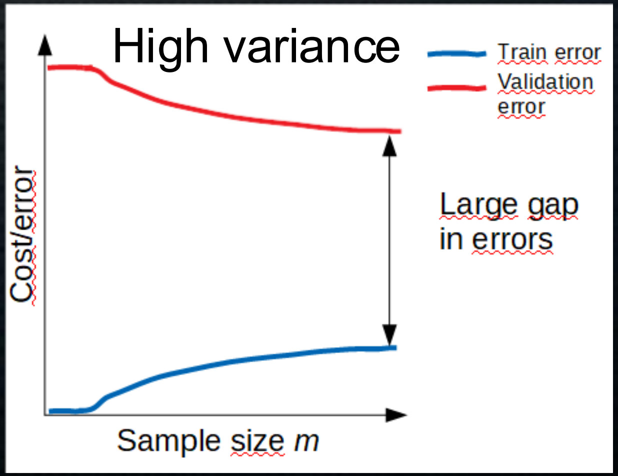
- Data is split into data to train on and a test set that you don‘t touch at all
- Training data is split into k folds, with (average) cross-validation error as proxy for how your algorithm performs on unseen data

Summary: cross-validation and learning curves

- Data is split into data to train on and a test set that you don‘t touch at all
- Training data is split into k folds, with (average) cross-validation error as proxy for how your algorithm performs on unseen data
- Learning curves allow you to diagnose whether your algorithm suffers from high bias or high variance



Underfitting: use more complex model



Overfitting: use less complex model or supply more training data

Knock-knock: it’s reality, and it’s complex

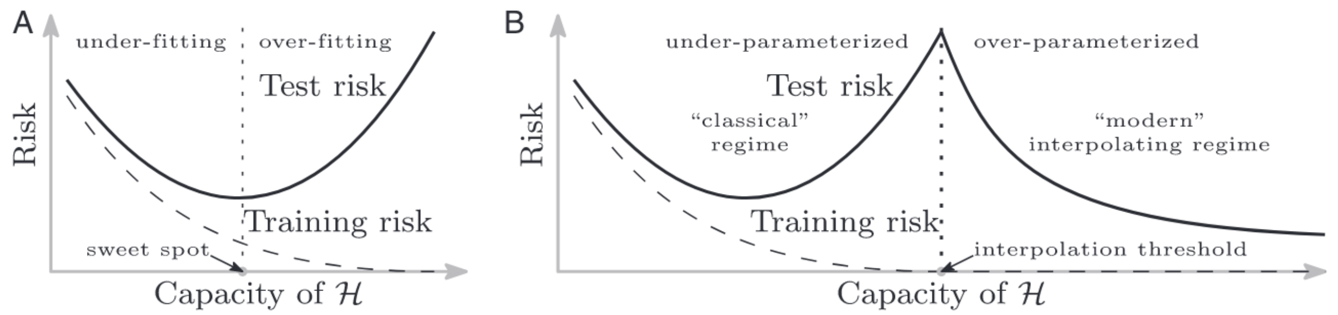


Fig. 1. Curves for training risk (dashed line) and test risk (solid line). (*A*) The classical U-shaped risk curve arising from the bias–variance trade-off. (*B*) The double-descent risk curve, which incorporates the U-shaped risk curve (i.e., the “classical” regime) together with the observed behavior from using high-capacity function classes (i.e., the “modern” interpolating regime), separated by the interpolation threshold. The predictors to the right of the interpolation threshold have zero training risk.

Belkin, M., Hsu, D., Ma, S., & Mandal, S. (2019). Reconciling modern machine-learning practice and the classical bias–variance trade-off. *Proceedings of the National Academy of Sciences*, *116*(32), 15849-15854.

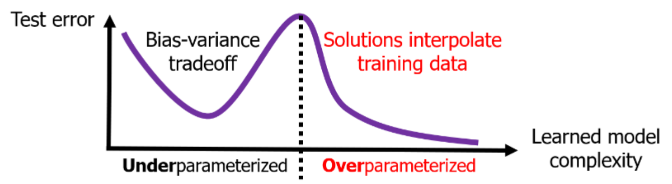


Figure 1: Double descent of test errors (i.e., generalization errors) with respect to the complexity of the learned model. TOPML studies often consider settings in which the learned model complexity is expressed as the number of (independently tunable) parameters in the model. In this qualitative demonstration, the global minimum of the test error is achieved by maximal overparameterization.

Dar, Y., Muthukumar, V., & Baraniuk, R. G. (2021). A farewell to the bias-variance tradeoff? an overview of the theory of overparameterized machine learning. *arXiv preprint arXiv:2109.02355*.

Belkin, M. (2021). Fit without fear: remarkable mathematical phenomena of deep learning through the prism of interpolation. *Acta Numerica*, *30*, 203-248.

What can we do to find a good model?

- ~~Find a way to approximate generalisation error: how well do you do on unseen data?~~
- ~~See how error on seen and unseen data changes with amount of training data (plot learning curves)~~
- ***Automatically constrain the fitting by penalising the cost function for too many/too large parameters → I will tell you tomorrow!***

Summary

- We want our models to **generalise well** but have to contend with **bias** and **variance**
- We can measure (by proxy) how well we generalise using cross-validation
- We can plot learning curves for different subsamplings of the data to diagnose bias and variance.
  - High bias: data doesn't help performance
  - High variance: more data helps