# CS-567 Machine Learning

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Lectures 2 and 3
Curve Fitting and Regularization
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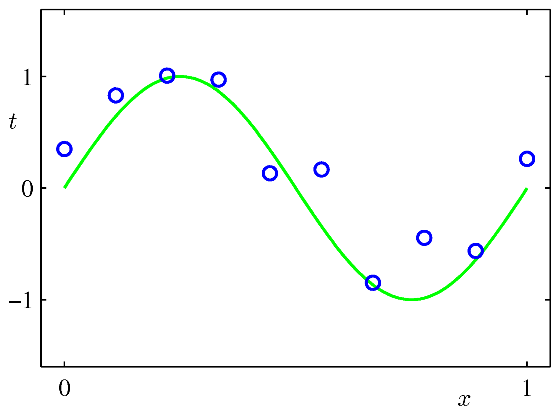
# Example: Polynomial Curve Fitting

**Problem**: Given $N$ observations of input $x_i$ with corresponding observations of output $t_i$, find function $f(x)$ that predicts $t$ for a new value of $x$.



First, let's generate some data.

```
N=10;
x=0:1/(N-1):1;
t=sin(2*pi*x);
plot(x,t,'o');
```

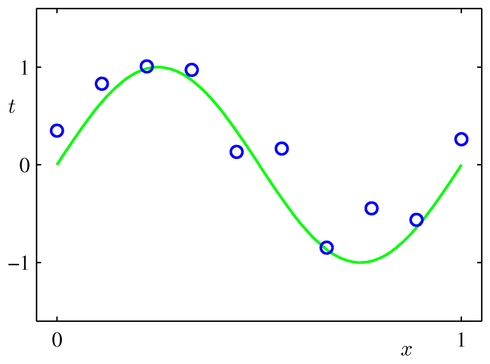
Notice that the data is generated through the function $\sin(2\pi x)$.
Real-world observations are always 'noisy'.
Let's add some noise to the data

```
n=randn(1,N)*0.3;
t=t+n;
plot(x,t,'o');
```

# Real-world Data

Real-world data has 2 important properties

1. underlying regularity,
2. individual observations are corrupted by noise.




Learning corresponds to discovering the underlying regularity of data (the $\sin(\cdot)$ function in our example).

# Polynomial curve fitting

- We will fit the points $(x, t)$ using a polynomial function

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

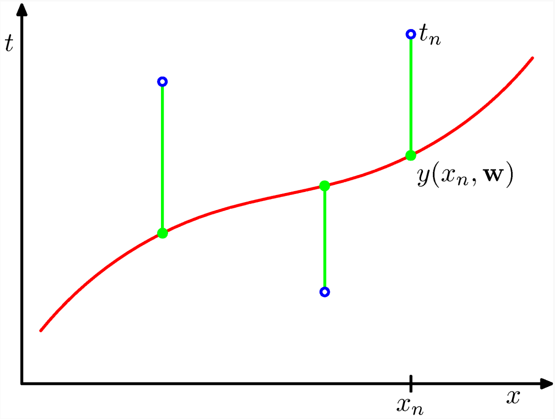
  where $M$ is the *order* of the polynomial.
- Function $y(x, \mathbf{w})$ is a
  - non-linear function of the input $x$, but
  - a linear function of the parameters $\mathbf{w}$.
- So our model $y(x, \mathbf{w})$ is a *linear model*.

# Polynomial curve fitting

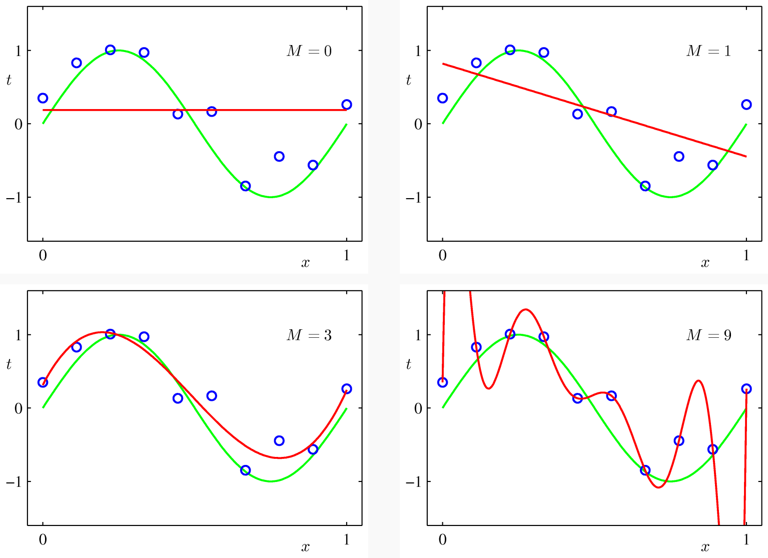
- Fitting corresponds to finding the optimal $\mathbf{w}$. We denote it as $\mathbf{w}^*$.
- Optimal $\mathbf{w}^*$ can be found by *minimising* an *error function*

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

- Why does minimising $E(\mathbf{w})$ make sense?
- Can $E(\mathbf{w})$ ever be negative?
- Can $E(\mathbf{w})$ ever be zero?




Geometric interpratation of the sum-of-squares error function.


M = 0
M = 1
M = 3
M = 9
t
x
1
0
−1
0
1

# Over-fitting

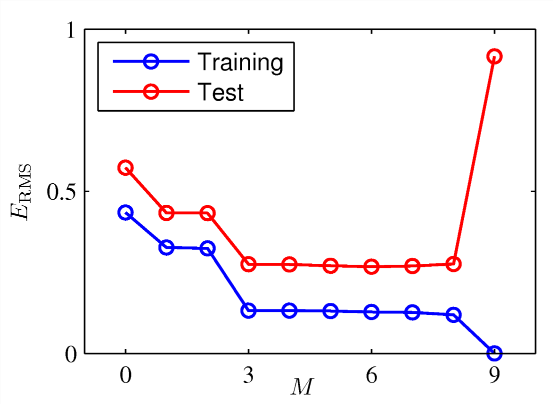
- Lower order polynomials can't capture the variation in data.
- Higher order leads to *over-fitting*.
  - Fitted polynomial passes *exactly* through each data point.
  - But it oscillates wildly in-between.
  - Gives a very poor representation of the real underlying function.
- Over-fitting is bad because it gives bad generalization.

# Over-fitting

- To check generalization performance of a certain $\mathbf{w}^*$, compute $E(\mathbf{w}^*)$ on a *new* test set.
- Alternative performance measure: root-mean-square error (RMS)

$$E_{RMS} = \sqrt{\frac{2E(\mathbf{w}^*)}{N}}$$

- Mean ensures datasets of different sizes are treated equally. (How?)
- Square-root brings the *squared* error scale back to the scale of the target variable $t$.




Root-mean-square error on training and test set for various polynomial orders M.

# Paradox?

- A polynomial of order $M$ contains all polynomials of lower order.
- So higher order should *always* be better than lower order.
- **But**, it's not better. Why?
    - Because higher order polynomial starts fitting the noise instead of the underlying function.

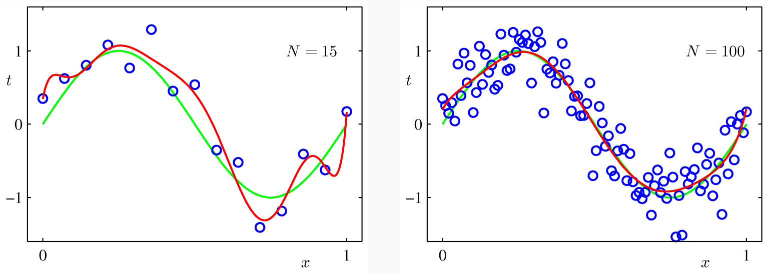
# Over-fitting

| | $M=0$ | $M=1$ | $M=3$ | $M=9$ |
|---|---|---|---|---|
| $w_0^\star$ | 0.19 | 0.82 | 0.31 | 0.35 |
| $w_1^\star$ | | -1.27 | 7.99 | 232.37 |
| $w_2^\star$ | | | -25.43 | -5321.83 |
| $w_3^\star$ | | | 17.37 | 48568.31 |
| $w_4^\star$ | | | | -231639.30 |
| $w_5^\star$ | | | | 640042.26 |
| $w_6^\star$ | | | | -1061800.52 |
| $w_7^\star$ | | | | 1042400.18 |
| $w_8^\star$ | | | | -557682.99 |
| $w_9^\star$ | | | | 125201.43 |

- Typical magnitude of the polynomial coefficients is increasing dramatically as $M$ increases.
- This is a sign of over-fitting.
- The polynomial is trying to fit the data points exactly by having larger coefficients.

# Over-fitting

- Large $M \implies$ more flexibility $\implies$ more tuning to noise.
- **But**, if we have more data, then over-fitting is reduced.




- Fitted polynomials of order $M = 9$ with $N = 15$ and $N = 100$ data points. More data reduces the effect of over-fitting.
- Rough heuristic to avoid over-fitting: Number of data points should be greater than $k|\mathbf{w}|$ where $k$ is some multiple like 5 or 10.

# How to avoid over-fitting

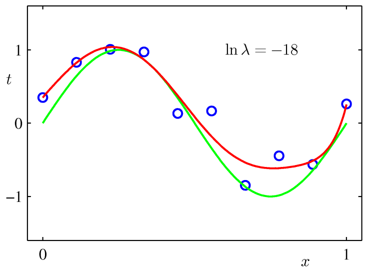
- Since large coefficients $\implies$ over-fitting, *discourage large coefficents* in $\mathbf{w}$.

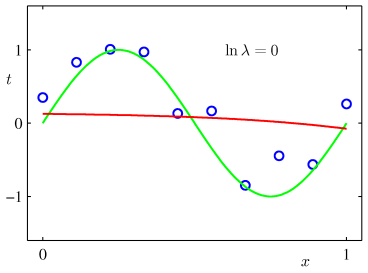
$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$

  where $||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w} = w_0^2 + w_1^2 + \cdots + w_M^2$ and $\lambda$ controls the relative importance of the regularizer compared to the error term.

- Also called *regularization, shrinkage, weight-decay*.

For a polynomial of order 9



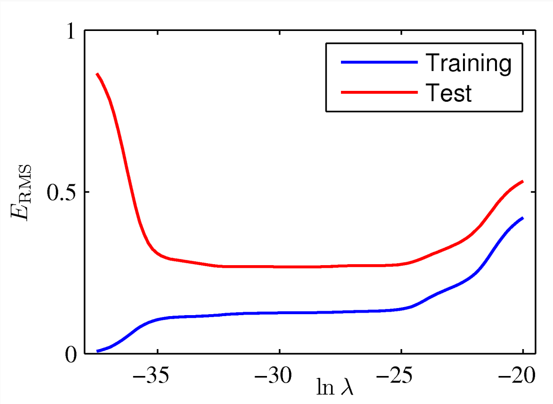

For $\lambda = e^{-18}$
No over-fitting

For $\lambda = 1$
Too much smoothing (no fitting)

# Effect of regularization

| | $\ln \lambda = -\infty$ | $\ln \lambda = -18$ | $\ln \lambda = 0$ |
|---|---|---|---|
| $w_0^\star$ | 0.35 | 0.35 | 0.13 |
| $w_1^\star$ | 232.37 | 4.74 | -0.05 |
| $w_2^\star$ | -5321.83 | -0.77 | -0.06 |
| $w_3^\star$ | 48568.31 | -31.97 | -0.05 |
| $w_4^\star$ | -231639.30 | -3.89 | -0.03 |
| $w_5^\star$ | 640042.26 | 55.28 | -0.02 |
| $w_6^\star$ | -1061800.52 | 41.32 | -0.01 |
| $w_7^\star$ | 1042400.18 | -45.95 | -0.00 |
| $w_8^\star$ | -557682.99 | -91.53 | 0.00 |
| $w_9^\star$ | 125201.43 | 72.68 | 0.01 |

- As $\lambda$ increases, the typical magnitude of coefficients gets smaller.
- We go from over-fitting ($\lambda = 0$) to no over-fitting ($\lambda = e^{-18}$) to poor fitting ($\lambda = 1$).
- Since $M = 9$ is fixed, regularization controls the degree of over-fitting.




Graph of root-mean-square (RMS) error of fitting the $M = 9$ polynomial as $\lambda$ is increased.

# How to avoid over-fitting

- A more principled approach to control over-fitting is the *Bayesian approach* (to be covered later).
  - Determines the *effective* number of parameters automatically.
- We need the machinery of *probability* to understand the Bayesian approach.
- Probability theory also offers a more principled approach for our polynomial fitting example.
- Will be covered in the next lecture.