CS-453 Machine Learning

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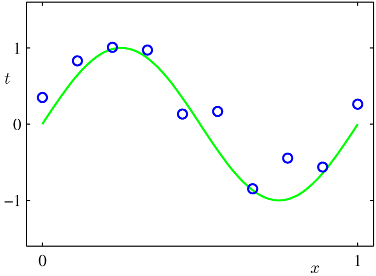
2. Curve Fitting and Regularization

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');
```

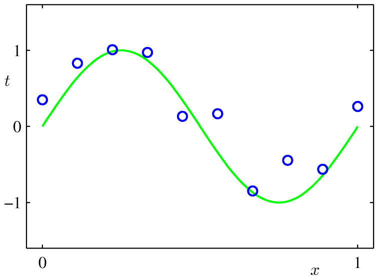
Notice that the data is generated through the function $\sin(2\pi x)$. Real-world observations are always 'noisy'.
Let's add some noise to the data

```
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

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

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

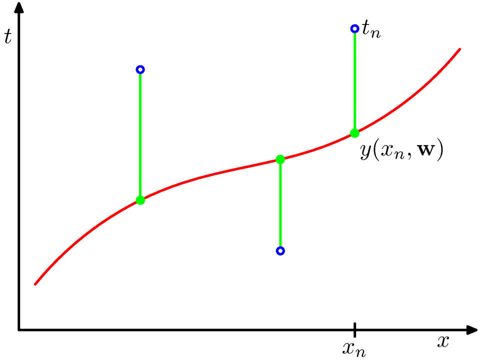
Polynomial curve fitting

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

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

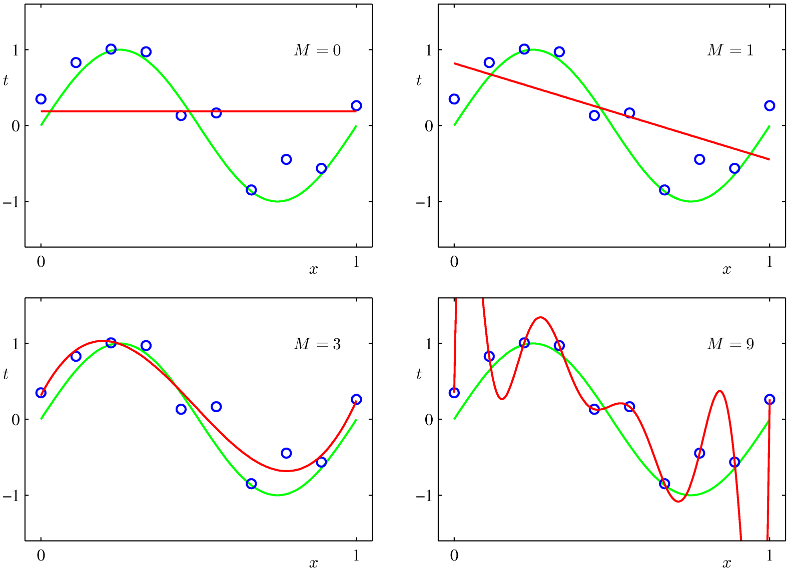
- Why does minimising $E(\mathrm{w})$ make sense?
- Can $E(\mathrm{w})$ ever be negative?
- Can $E(\mathrm{w})$ ever be zero?

Geometric Interpretation



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

Power of a polynomial



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*.
  - Generalization refers to performance on unseen data.

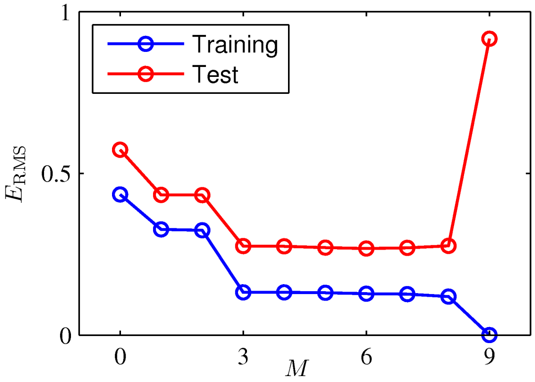
Over-fitting

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

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

- 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.

Over-fitting



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.

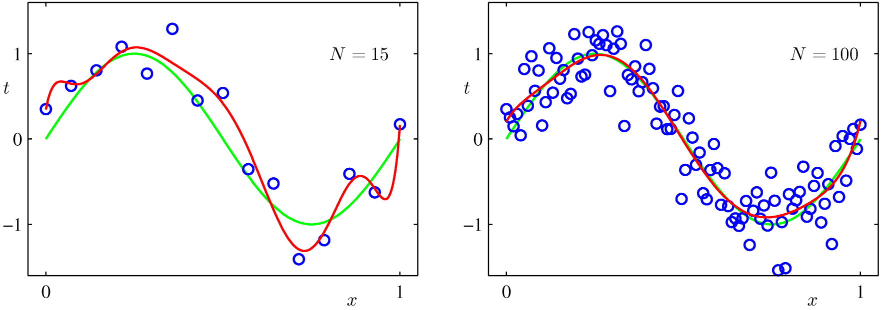
Over-fitting

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	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 $k|\mathrm{w}|$ where k is some multiple like 5 or 10.

How to avoid over-fitting

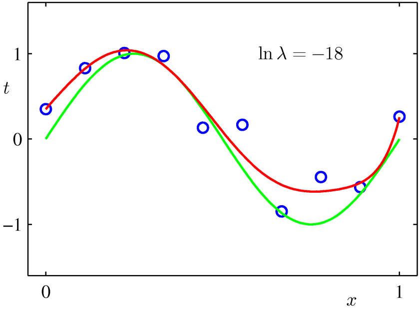
- Since large coefficients $\implies$ over-fitting, *discourage large coefficents* in w.

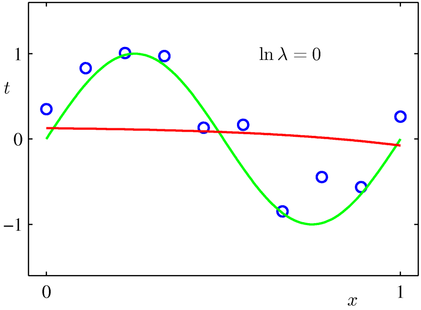
$$\tilde{E}(\mathrm{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathrm{w}) - t_n\}^2 + \frac{\lambda}{2}||\mathrm{w}||^2$$

  where $||\mathrm{w}||^2 = \mathrm{w}^T\mathrm{w} = w_0^2 + w_1^2 + \cdots + w_M^2$ and λ controls the relative importance of the regularizer compared to the error term.
- Also called *regularization, shrinkage, weight-decay*.

How to avoid over-fitting

For a polynomial of order 9





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

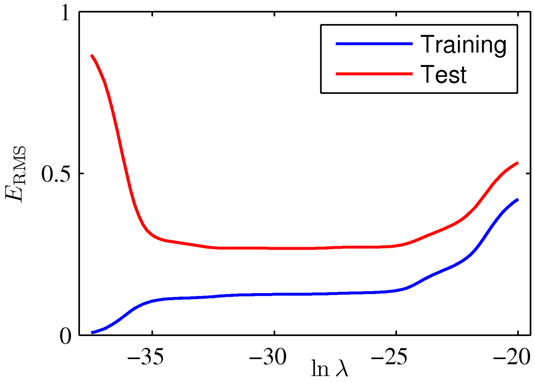
For $\lambda = 1$
Too much smoothing (no fitting)

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 λ 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.

Effect of regularization



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