Lecture 3: Under-fitting, Over-fitting, Regularization, and Model Selection

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

Reading materials

- Chapter 3.1 & 3.2, Bishop, Pattern Recognition and Machine Learning
- Read about over-fitting in the paper by Pedro Domingos (Sections 3 and 5 of “A few useful things to know about machine learning”)

Reference

- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

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Definition 1 (*Learning* problem can be formulated as optimization problem)

Given a cost function $\mathcal{L}(\mathbf{w})$, we wish to find $\mathbf{w}^\star$ which minimizes the cost:

$$\min_{\mathbf{w}} \; \mathcal{L}(\mathbf{w}) \quad \text{subject to } \mathbf{w} \in \mathbb{R}^D \tag{1}$$

We will use an optimization algorithm (e.g., Gradient Descent) to find a good $\mathbf{w}$.

Considering a dataset $\mathcal{D} = \{\mathbf{X}, \mathbf{y}\}$ and learnable weights $\mathbf{w} \in \mathbb{R}^D$ for $f_{\mathbf{w}}(\mathbf{X}) = \mathbf{X}\mathbf{w}$.

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N, \qquad \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix} \in \mathbb{R}^{N\times D} \tag{2}$$

Using Gradient Descent for Linear Regression with MSE

The MSE is defined as:

$$\mathcal{L}(\mathbf{w}) := \frac{1}{2N} \sum_{n=1}^{N} \left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \tfrac{1}{2N} \mathbf{e}^\top \mathbf{e} \,. \tag{3}$$

The error vector $\mathbf{e}$ is defined as:

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w} = \begin{pmatrix} e_1 \\ \vdots \\ e_N \end{pmatrix} \in \mathbb{R}^N \,, \tag{4}$$

where $e_i := y_n - \mathbf{x}_n^\top \mathbf{w}$.

The gradient is given by

$$\nabla \mathcal{L}(\mathbf{w}) = -\tfrac{1}{N} \mathbf{X}^\top \mathbf{e} \tag{5}$$

A probabilistic model for linear regression

Definition 2 (Data generation process)

We assume that the data is generated by the model,

$$y_n = \mathbf{x}_n^\top \mathbf{w} + \epsilon_n, \tag{6}$$

where

- the ϵ_n (the noise) is a zero-mean Gaussian random variable with variance σ^2
- the noise is independent of each other and independent of the input.
- the model $\mathbf{w}$ is unknown.

The likelihood of the data vector $\mathbf{y} = (y_1, \cdots, y_N)$ given the input $\mathbf{X}$ and the model $\mathbf{w}$ is

$$p(\mathbf{y} \,|\, \mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} p(y_n \,|\, \mathbf{x}_n, \mathbf{w}) = \prod_{n=1}^{N} \mathcal{N}(y_n \,|\, \mathbf{x}_n^\top \mathbf{w}, \sigma^2). \tag{7}$$

The probabilistic view point: maximize this likelihood over the choice of model $\mathbf{w}$.

Maximum-Likelihood Estimator (MLE)

Instead of maximizing the likelihood, we can maximize the logarithm of the likelihood, i.e., log-likelihood (LL):

$$\mathcal{L}_{\text{LL}}(\mathbf{w}) := \log\, p(\mathbf{y} \,|\, \mathbf{X}, \mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst.} \tag{8}$$

Compare the LL to the MSE (Mean Squared Error)

$$\mathcal{L}_{\text{LL}}(\mathbf{w}) = -\frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \text{cnst} \tag{9}$$

$$\mathcal{L}_{\text{MSE}}(\mathbf{w}) = \frac{1}{2N} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 \tag{10}$$

Maximizing the LL is equivalent to minimizing the MSE:

$$\arg\min_{\mathbf{w}}\, \mathcal{L}_{\text{MSE}}(\mathbf{w}) = \arg\max_{\mathbf{w}}\, \mathcal{L}_{\text{LL}}(\mathbf{w}). \tag{11}$$

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Motivation

- In rare cases, one can compute the optimum of the cost function analytically.
- Linear regression using an MSE cost function is one such case.
- Here its solution can be obtained explicitly, by solving a linear system of equations.

$\Rightarrow$ These equations are sometimes called the normal equations.

$\Rightarrow$ Solving the normal equations is called the least squares.

Normal Equations

To derive the normal equations,

1. we first show that the problem is convex.

2. we then use the optimality conditions for convex functions, i.e.,

$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0}\,, \tag{12}$$

   where $\mathbf{w}^\star$ corresponds to the parameter at the optimum point.

   Given the definition $\mathcal{L}(\mathbf{w}) = \frac{1}{2N}\sum_{n=1}^{N}\left(y_n - \mathbf{x}_n^\top \mathbf{w}\right)^2 = \frac{1}{2N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})$, we have

$$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N}\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = 0\,, \tag{13}$$

   where we can get the normal equations for linear regression.

Least Squares

We need to solve the linear system of the normal equation $\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$, where

$$\mathbf{X}^\top y = \underbrace{\mathbf{X}^\top\mathbf{X}}_{\text{Gram matrix}} \mathbf{w} \tag{14}$$

If the Gram matrix is invertible, we can multiply the normal equation by the inverse of the Gram matrix from the left:

$$\mathbf{w}^\star = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}\,, \tag{15}$$

where we can get a closed-form expression for the minimum.

Last lecture:

- Basic concept of regression and classification
- Linear regression
  - Definition
  - Gradient Descent (GD) optimization
  - Least Square
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This lecture:

- Over-fitting and Under-fitting
- Polynomial Regression, Ridge Regression, and Lasso Regression
- Generalization, and Model selection

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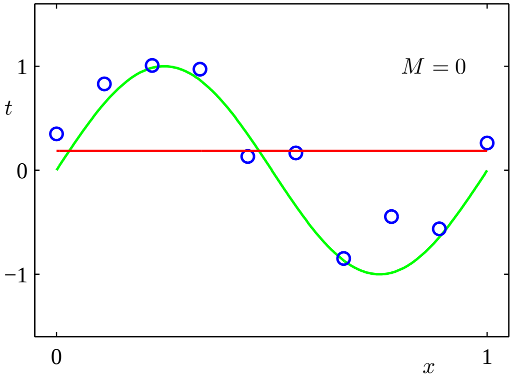
Under-fitting with Linear Models $f_{\mathbf{w}}(\mathbf{X}) := \mathbf{X}\mathbf{w}$



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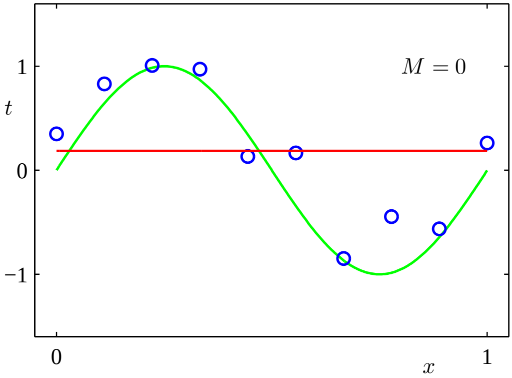

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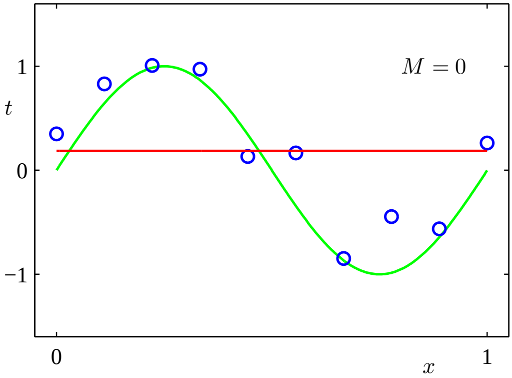

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- We do not observe $g(x_n)$ directly:

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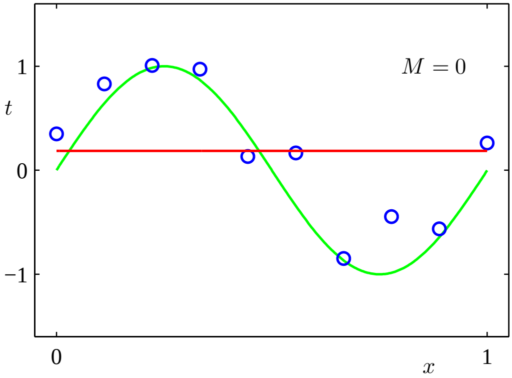

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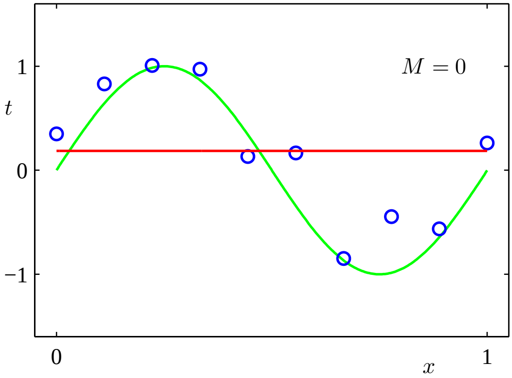

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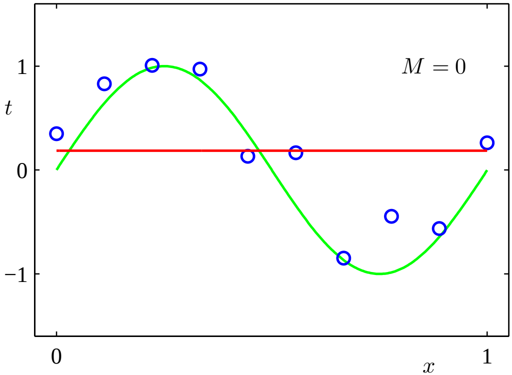

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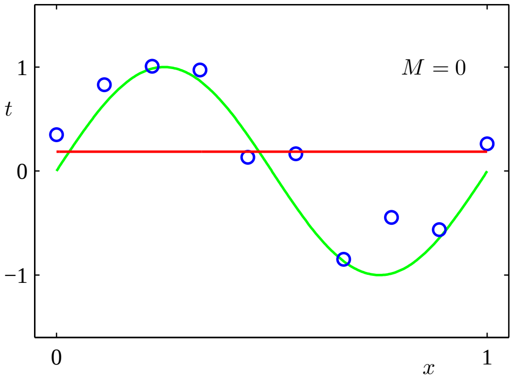

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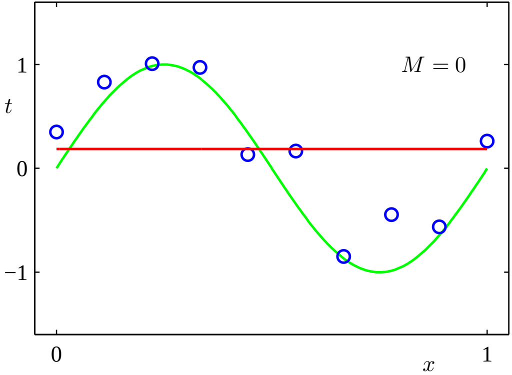

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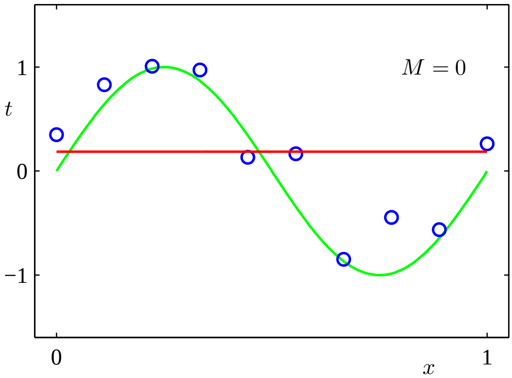

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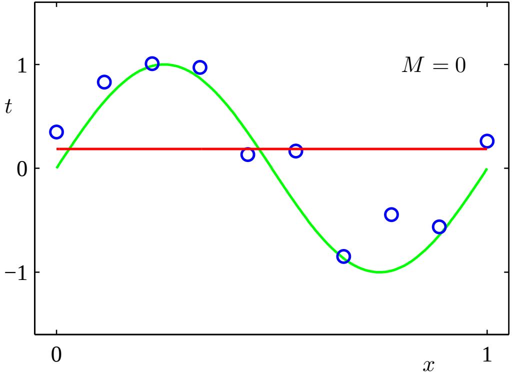

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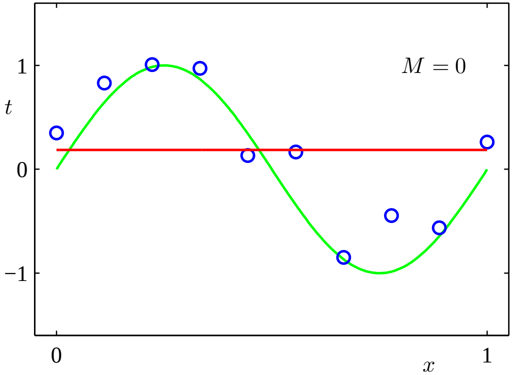

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Linear Model might under-fit!

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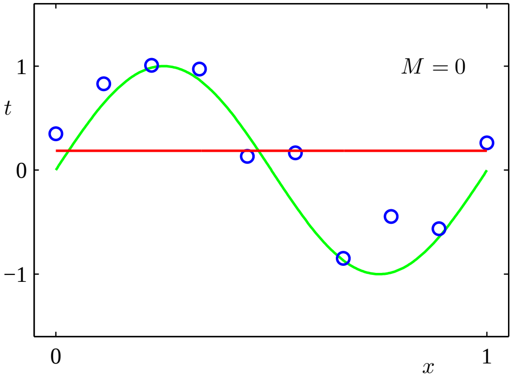

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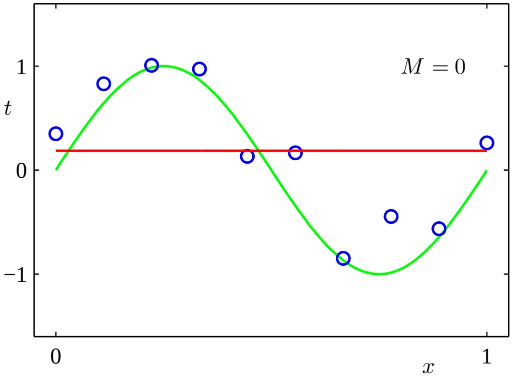

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Is it all good?

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Interpolation between under-fitting and over-fitting

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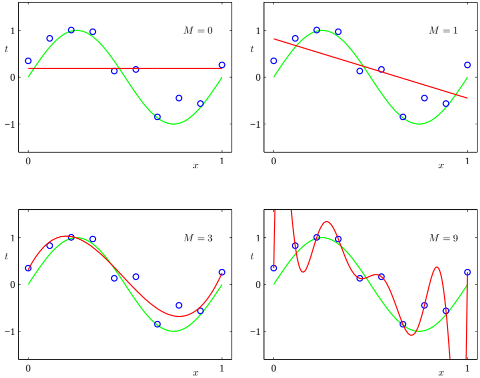

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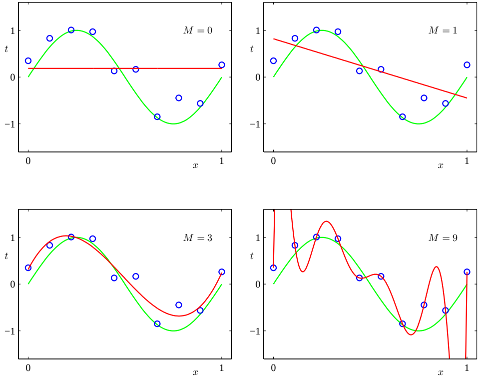

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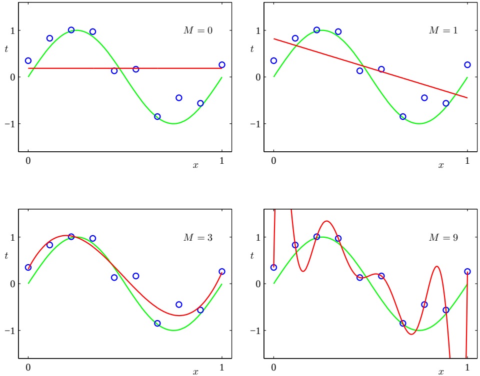

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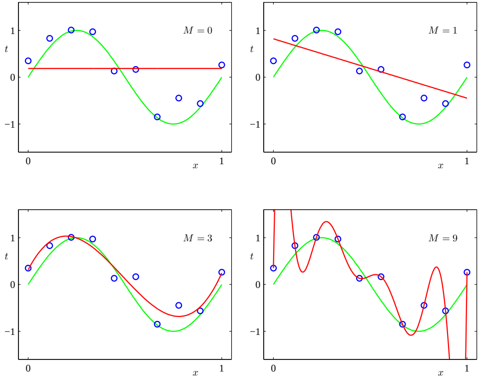

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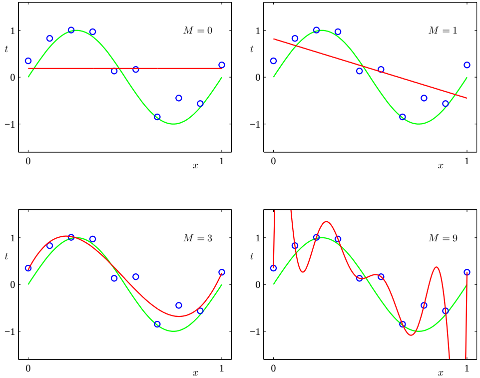

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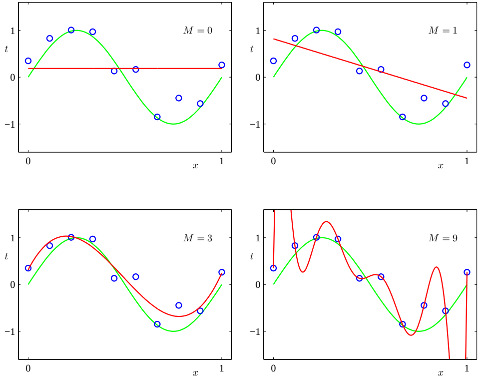

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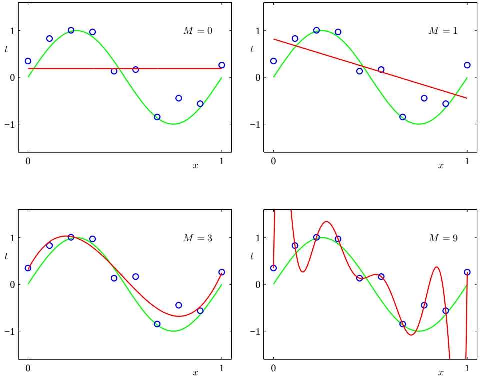

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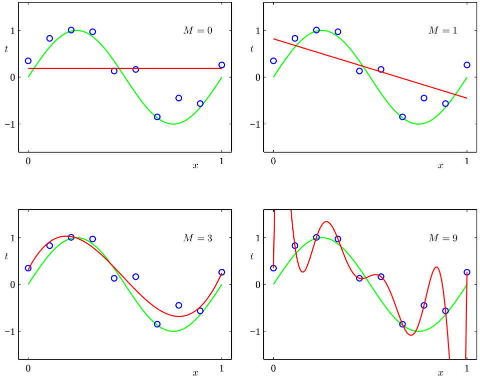

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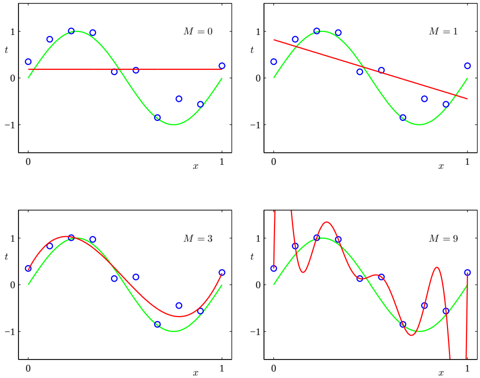

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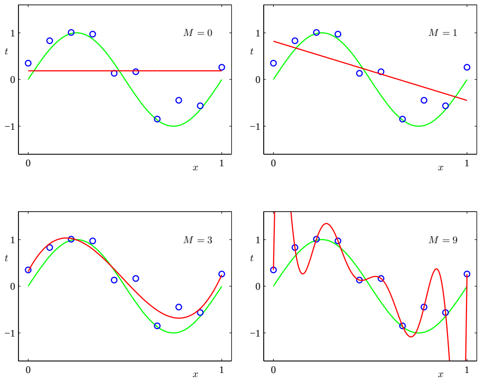
- For $M = 9$, the model fits every single points

Interpolation between under-fitting and over-fitting

Let's consider the polynomial regression problem (for a one-dimensional input feature x_n):

$$y_n \approx w_0 + w_1 x_n + w_2 x_n^2 + \ldots + w_M x_n^M =: \phi(x_n)^\top \mathbf{w} \,. \tag{21}$$



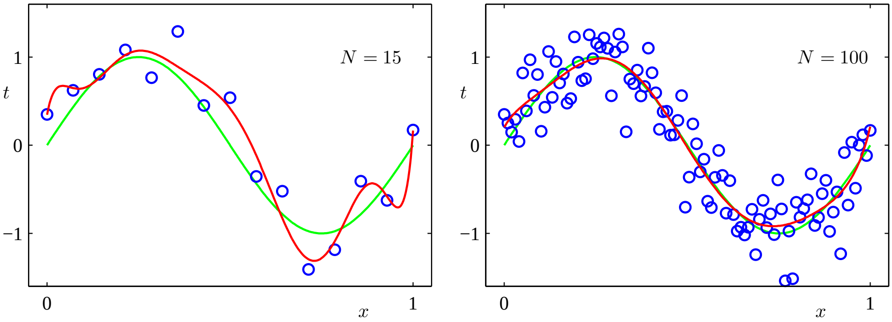
Settings:

- The circles are data points
- The green line represents the "true function"
- The red line is the learned model.

Observations:

- The model is under-fitting for $M = 0$ & $M = 1$
- For $M = 3$, the model fits the data
  $\rightarrow$ but can be improved
- For $M = 9$, the model fits every single points
  $\rightarrow$ severe over-fitting

- **Question:** How to avoid over-fitting?



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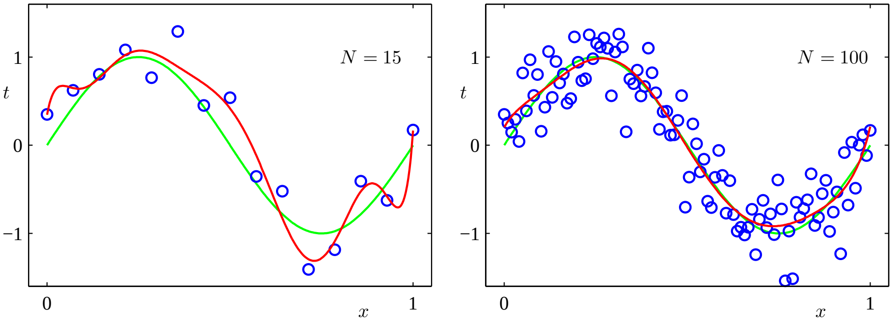

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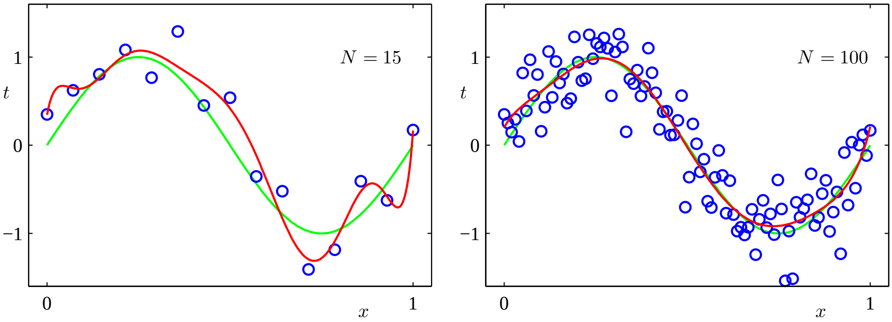

Increasing N but keeping M fixed.

We will elaborate on this question in the next section!

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We have seen that by augmenting the feature vector:

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Regularization is a way to mitigate this undesirable behavior.

- We will discuss regularization in the context of linear models
- The same principle applies also to more complex models such as neural nets.

Regularization

Through regularization, we can penalize complex models and favor simpler ones:

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- Model Complexity $\iff$ The richness of the model space.

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L_2-regularization: Ridge Regression

The most frequently used regularizer is the standard Euclidean norm (L_2-norm), which is

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- *Linear Regression* is a special case of this: by setting $\lambda := 0$.

Explicit solution of Ridge Regression for $\mathbf{w}$

Ridge Regression can be defined as:

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 \ + \ \lambda \|\mathbf{w}\|_2^2 \ . \tag{26}$$

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Differentiating and setting to zero (following a similar procedure as least squares):

$$\mathbf{w}^{\star}_{\text{ridge}} = (\mathbf{X}^{\top}\mathbf{X} + \lambda'\mathbf{I})^{-1}\mathbf{X}^{\top}\mathbf{y} \tag{27}$$

(here for simpler notation $\lambda'/2N = \lambda$)

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Write the Eigenvalue decomposition of $\mathbf{X}^\top\mathbf{X}$ as $\mathbf{USU}^\top$.

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$$\begin{aligned}\mathbf{X}^\top\mathbf{X} + \lambda'\mathbf{I} &= \mathbf{USU}^\top + \lambda'\mathbf{UIU}^\top && (28)\\ &= \mathbf{U}[\mathbf{S} + \lambda'\mathbf{I}]\mathbf{U}^\top. && (29)\end{aligned}$$

□

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We see now that every Eigenvalue is “lifted” by an amount λ'. $\square$

An alternative proof (optional reading).

Recall that for a symmetric matrix $\mathbf{A}$ we can also compute eigenvalues by looking at the so-called Rayleigh ratio,

$$R(\mathbf{A}, \mathbf{v}) = \frac{\mathbf{v}^\top \mathbf{A}\mathbf{v}}{\mathbf{v}^\top \mathbf{v}}. \tag{30}$$

Note that if $\mathbf{v}$ is an eigenvector with eigenvalue λ, then the Rayleigh coefficient indeed gives us λ.

We can find the smallest and largest eigenvalue by minimizing and maximizing this coefficient.

But note that if we apply this to the symmetric matrix $\mathbf{X}^\top \mathbf{X} + \lambda' \mathbf{I}$, then for any vector $\mathbf{v}$ we have

$$\frac{\mathbf{v}^\top (\mathbf{X}^\top \mathbf{X} + \lambda' \mathbf{I})\mathbf{v}}{\mathbf{v}^\top \mathbf{v}} \geq \frac{\lambda' \mathbf{v}^\top \mathbf{v}}{\mathbf{v}^\top \mathbf{v}} = \lambda' . \tag{31}$$

$\square$

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L_1-regularization: the Lasso

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- A very important case is the L_1-norm, leading to L_1-regularization.

In combination with the MSE cost function (i.e., L_2-norm), this is known as the Lasso:

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \sum_{n=1}^{N} \left[y_n - \mathbf{x}_n^\top \mathbf{w} \right]^2 + \lambda \left\| \mathbf{w} \right\|_1 \qquad \text{where } \left\| \mathbf{w} \right\|_1 := \sum_i |w_i| \,. \tag{32}$$

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Geometric interpretation for the Ridge Regression

Recall the definition of the Ridge Regression:

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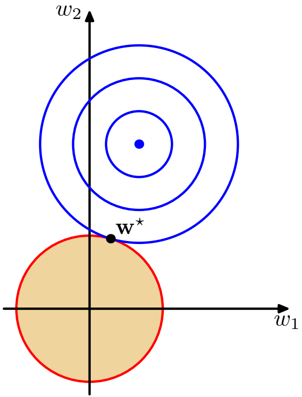

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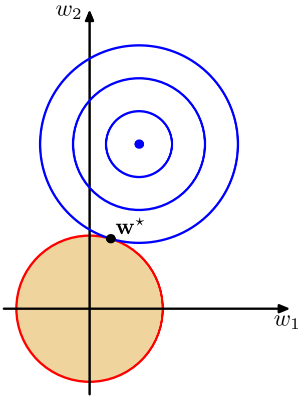

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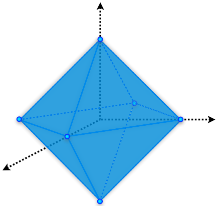

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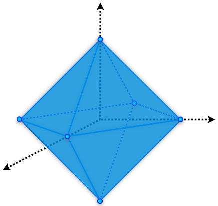

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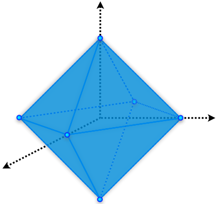

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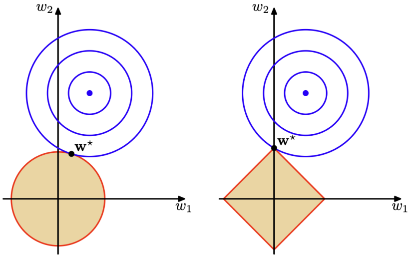

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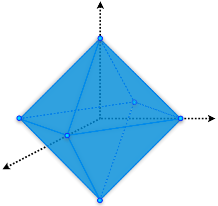

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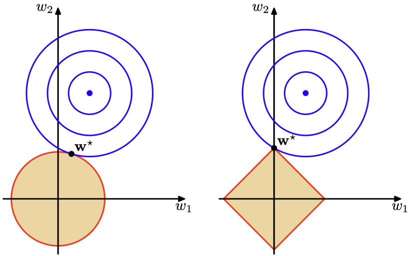

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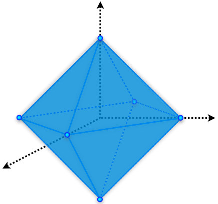

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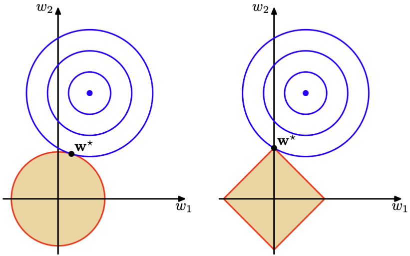

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- This forces some of the elements of $\mathbf{w}$ to be strictly 0.
- As λ is increased, an increasing number of parameters are driven to 0.

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The probabilistic interpretation of least-squares linear regression

Least-Squares linear regression can be interpreted as the Maximum Likelihood Estimator:

$$
\begin{aligned}
\mathbf{w}_{\text{lse}} &\overset{(a)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{y}, \mathbf{X}|\mathbf{w}) && \text{(by the definition of log-likelihood)}\\
&\overset{(b)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{X}|\mathbf{w}) p(\mathbf{y}|\mathbf{X}, \mathbf{w}) && \text{(by factoring the likelihood)}\\
&\overset{(c)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{X}) p(\mathbf{y}|\mathbf{X}, \mathbf{w}) && \text{(the choice of the input } \mathbf{x}_n \text{ is independent of } \mathbf{w})\\
&\overset{(d)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{y}|\mathbf{X}, \mathbf{w}) && (p(\mathbf{X}) \text{ is independent of } \mathbf{w})\\
&\overset{(e)}{=} \arg\min_{\mathbf{w}} \quad -\log \left[\prod_{n=1}^{N} p(y_n|\mathbf{x}_n, \mathbf{w})\right] && \text{(we assume samples are iid.)}\\
&= \arg\min_{\mathbf{w}} \quad \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 && \text{(by definition and calculus)}
\end{aligned}
$$

The probabilistic interpretation of Ridge Regression

We start with the posterior $p(\mathbf{w}|\mathbf{X}, \mathbf{y})$ and chose $\mathbf{w}$ to maximize this posterior.

The Maximum-A-Posteriori (MAP) estimate:

$$
\begin{aligned}
\mathbf{w}_{\text{ridge}} &= \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{w}|\mathbf{X}, \mathbf{y}) && \text{(by the definition of posterior)} \\
&\overset{(a)}{=} \arg\min_{\mathbf{w}} \quad -\log \frac{p(\mathbf{y}, \mathbf{X}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{y}, \mathbf{X})} && \text{(by the Bayes' law)} \\
&\overset{(b)}{=} \arg\min_{\mathbf{w}} \quad -\log p(\mathbf{y}, \mathbf{X}|\mathbf{w})p(\mathbf{w}) && \text{(eliminate quantities that do not depend on } \mathbf{w}\text{)} \\
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&= \arg\min_{\mathbf{w}} \quad \sum_{n=1}^{N} \frac{1}{2\sigma^2}(y_n - \mathbf{x}_n^\top \mathbf{w})^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2 . && (36)
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$$

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What is the model selection problem?

Recall the Ridge Regression problem:

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- Which λ should we use?

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How do we choose these hyper-parameters?

Model selection for neural networks

Optimization Algorithms?

SGD
Adam
Which step-size?
Which batch-size?
Which momentum?

Neural Architectures?

FullyConnected
ConvNet
ResNet
Transformer
Which width?
Which depth?
Batch normalization?

Regularizations?

Weight decay?
Dropout?
Early stopping?
Data augmentation?

To give a meaningful answer to the above questions,
we first need to specify our data model!

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- Can add a subscript $f_{S,\lambda}$ to indicate the model dependency (for Ridge Regression).

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- The reason that $L_S(f_S)$ might not be close to $L_{\mathcal{D}}(f_S)$ is of course over-fitting.

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Definition 4 (Generalization error)

The *generalization error* is given by

$$\left|L_{\mathcal{D}}(f) - L_{S_{\text{test}}}(f)\right|.$$

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Next lecture:

- Model Selection (contd)
- Bias-Variance Decomposition
- Multi-Layer Perceptron (MLP)
- Back-Propagation (BP)