Advanced Machine Learning
Lecture 2: Linear models

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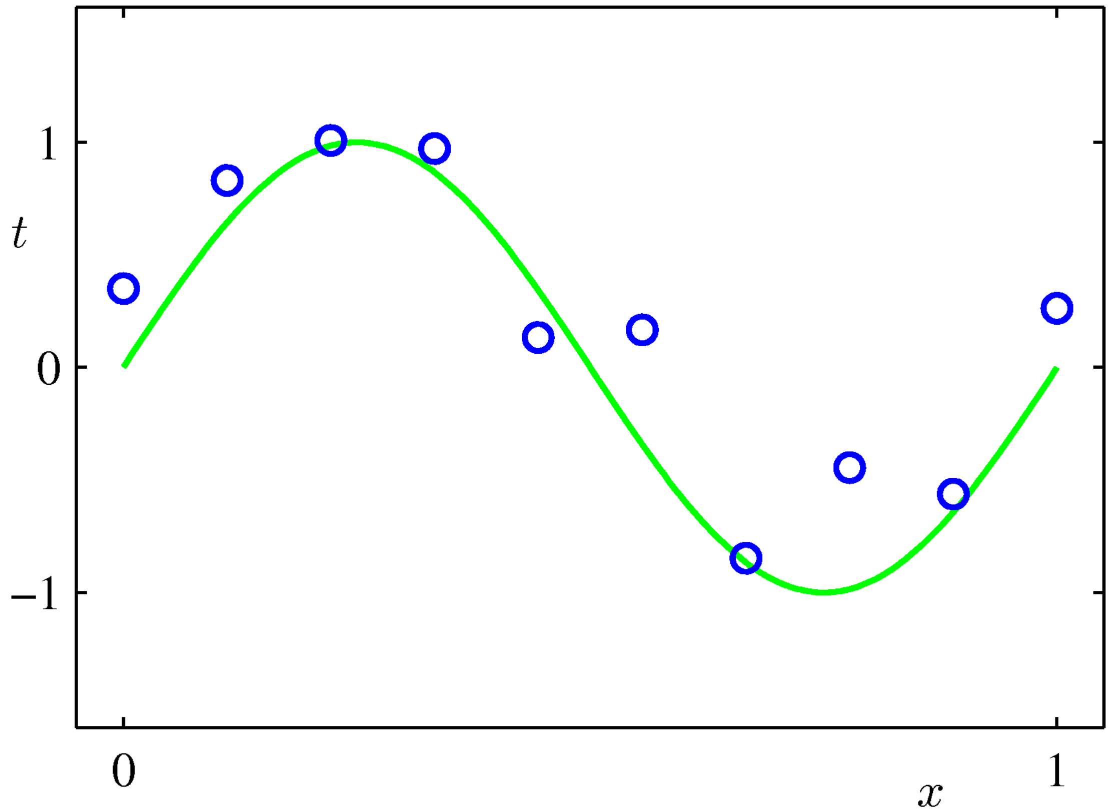
Linear models

Advanced Machine Learning

Polynomial curve fitting

- 10 points sampled from $\sin(2\pi x)$ + disturbance



$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} + \cdots$$

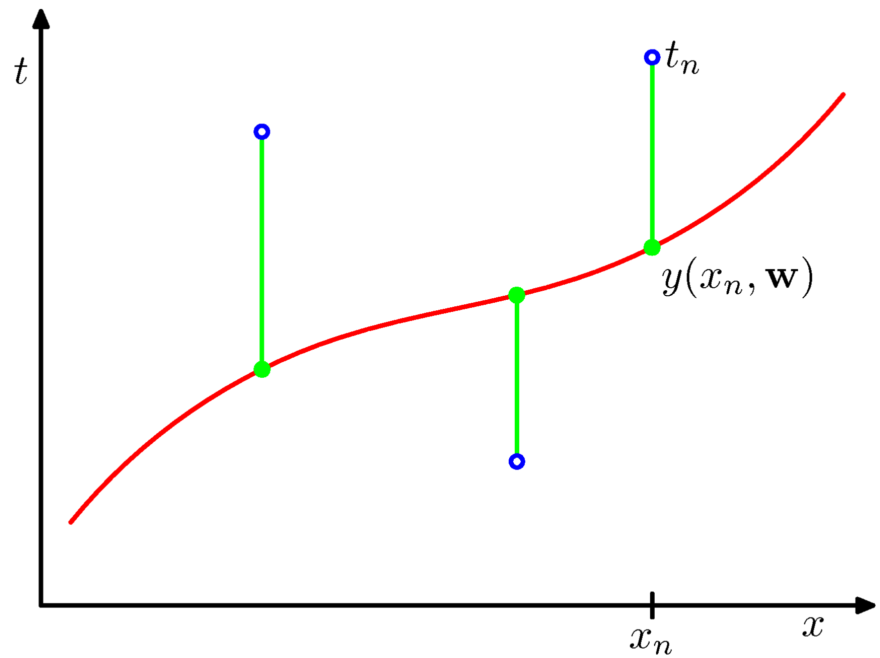
Polynomial curve fitting

- Polynomial curve

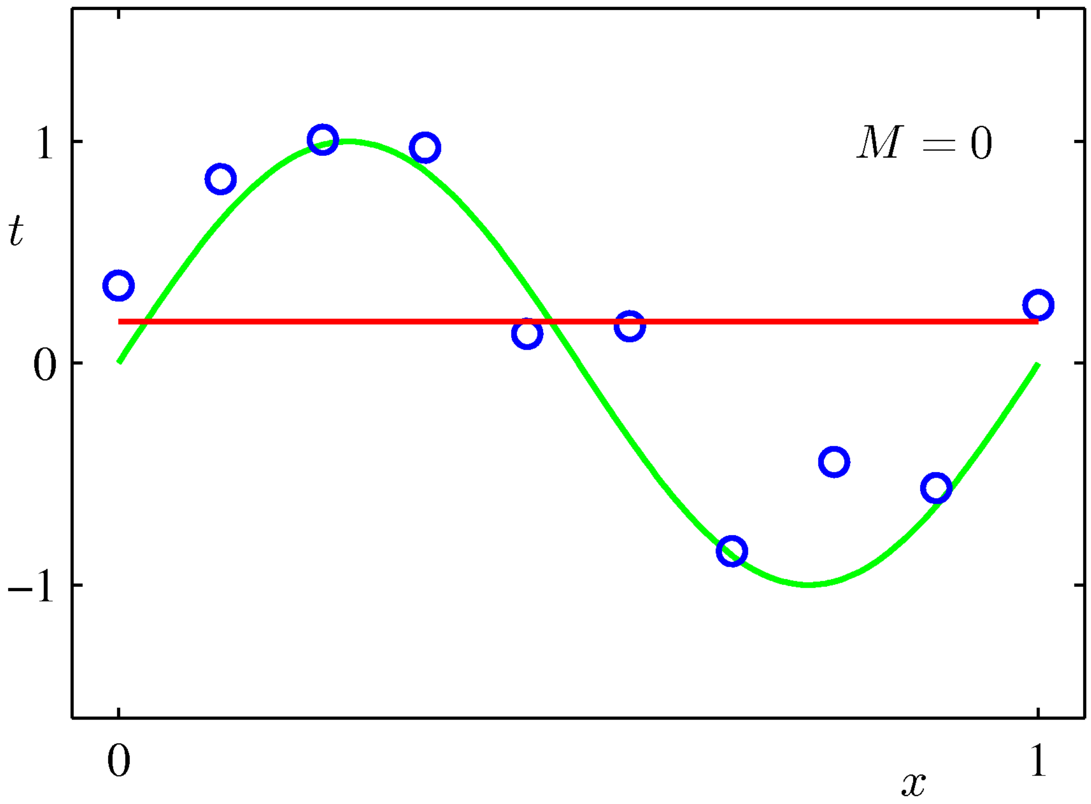
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

- Performance is measured by

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

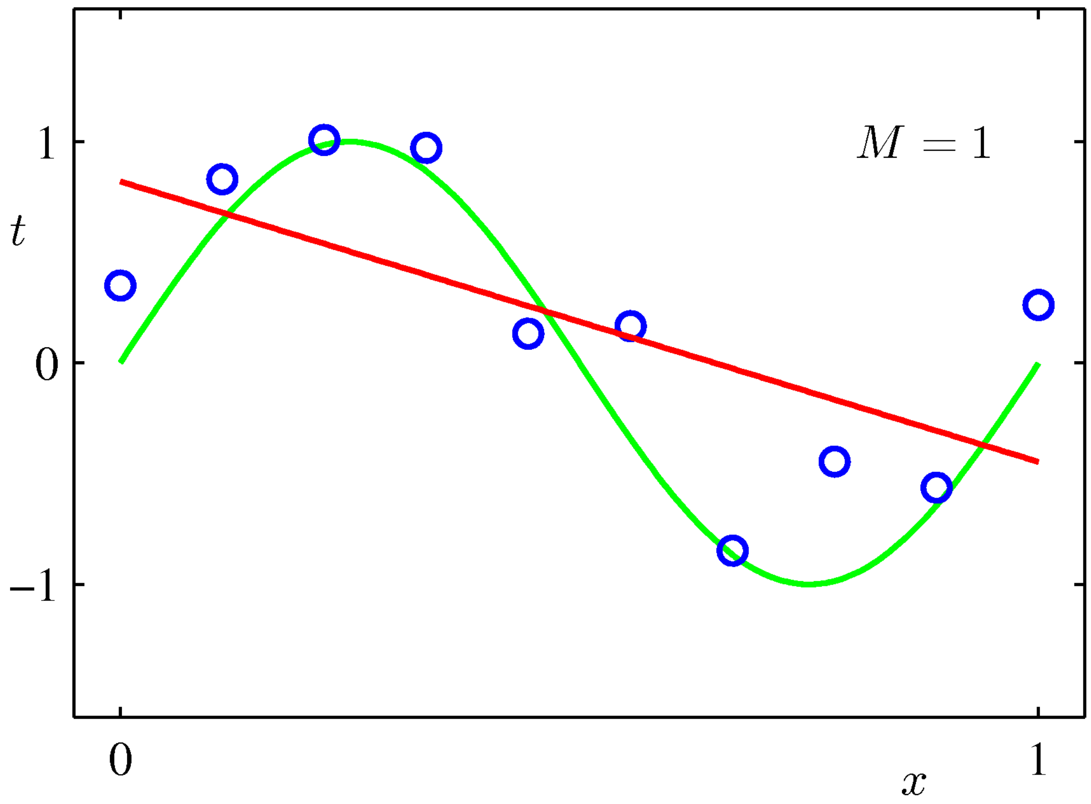


Polynomial curve fitting: order 0



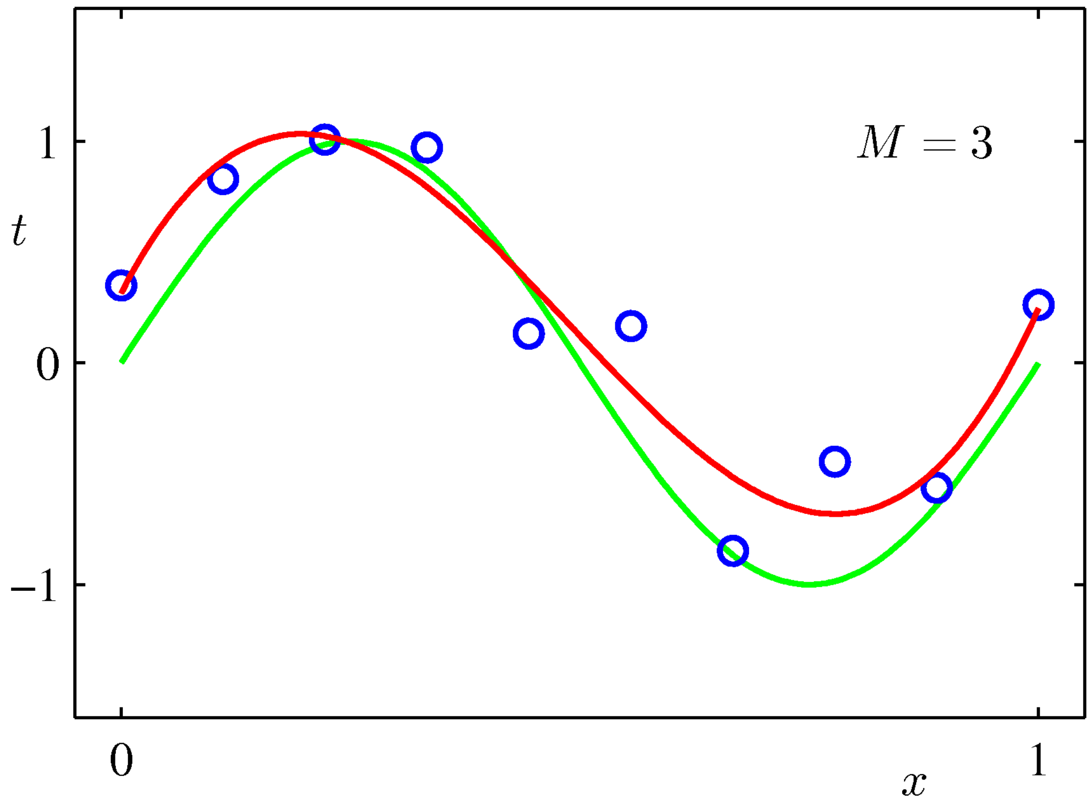
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Polynomial curve fitting: order 1



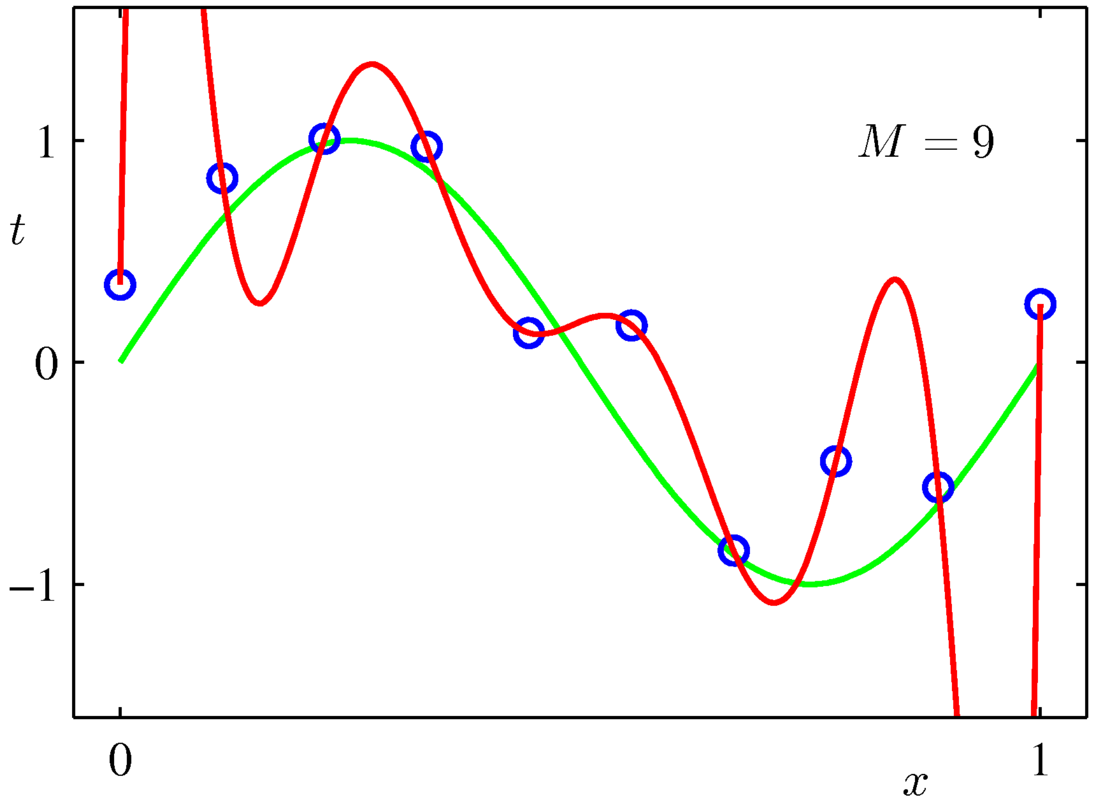
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Polynomial curve fitting: order 3



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

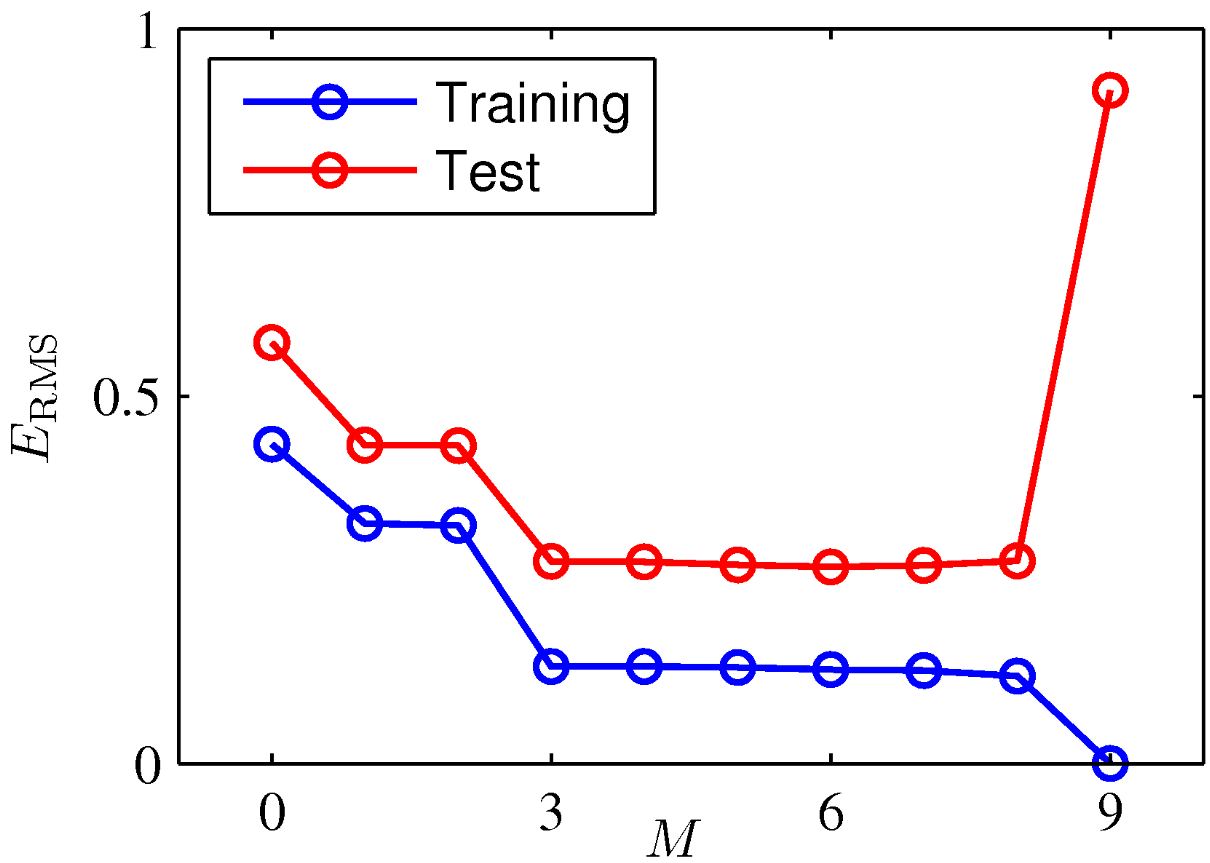
Polynomial curve fitting: order 9



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

Overfitting

- Root mean square (RMS) error: $E_{\text{RMS}} = \sqrt{2E(\mathbf{w}^*)/N}$

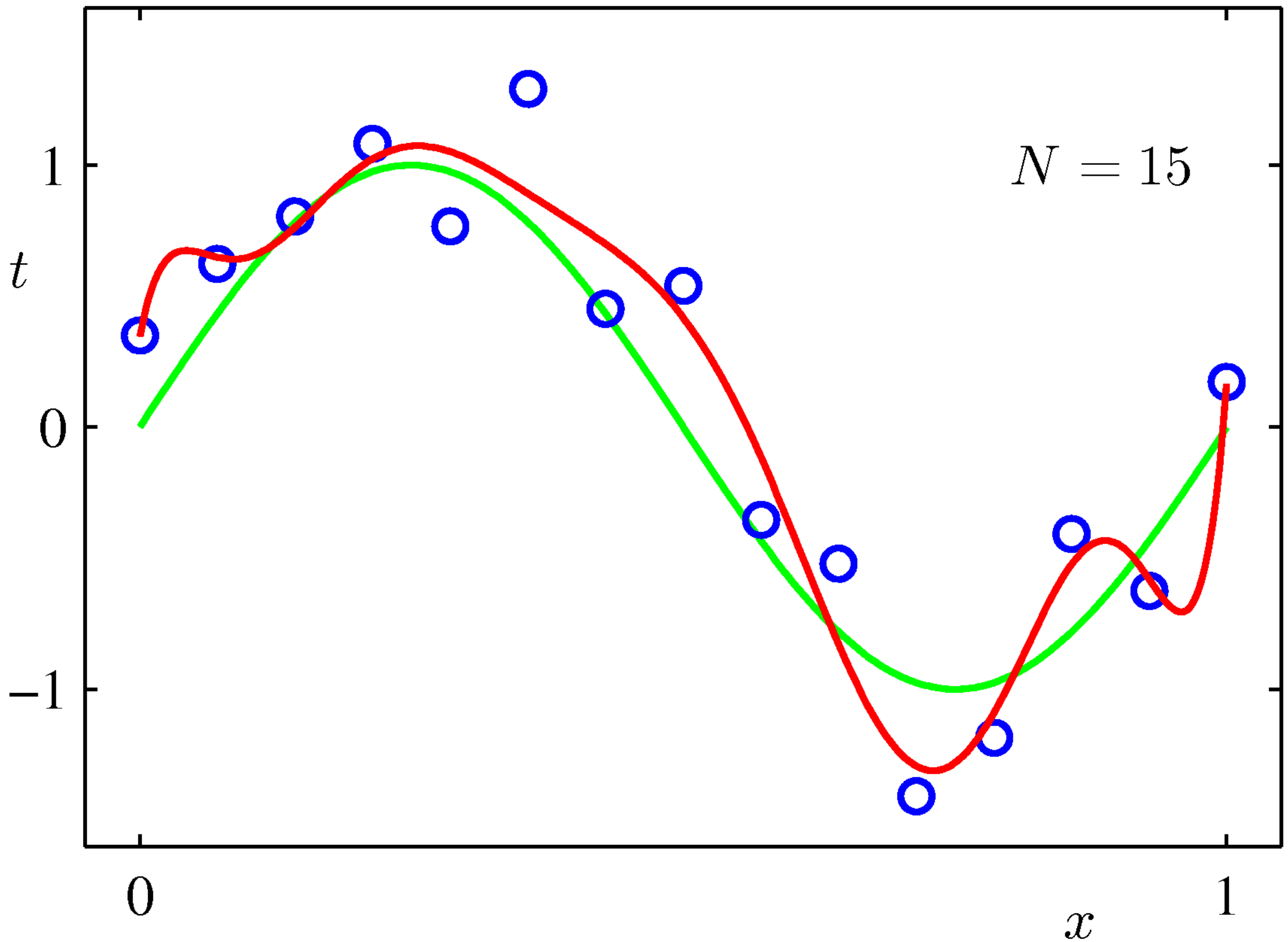


Overfitting

	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	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

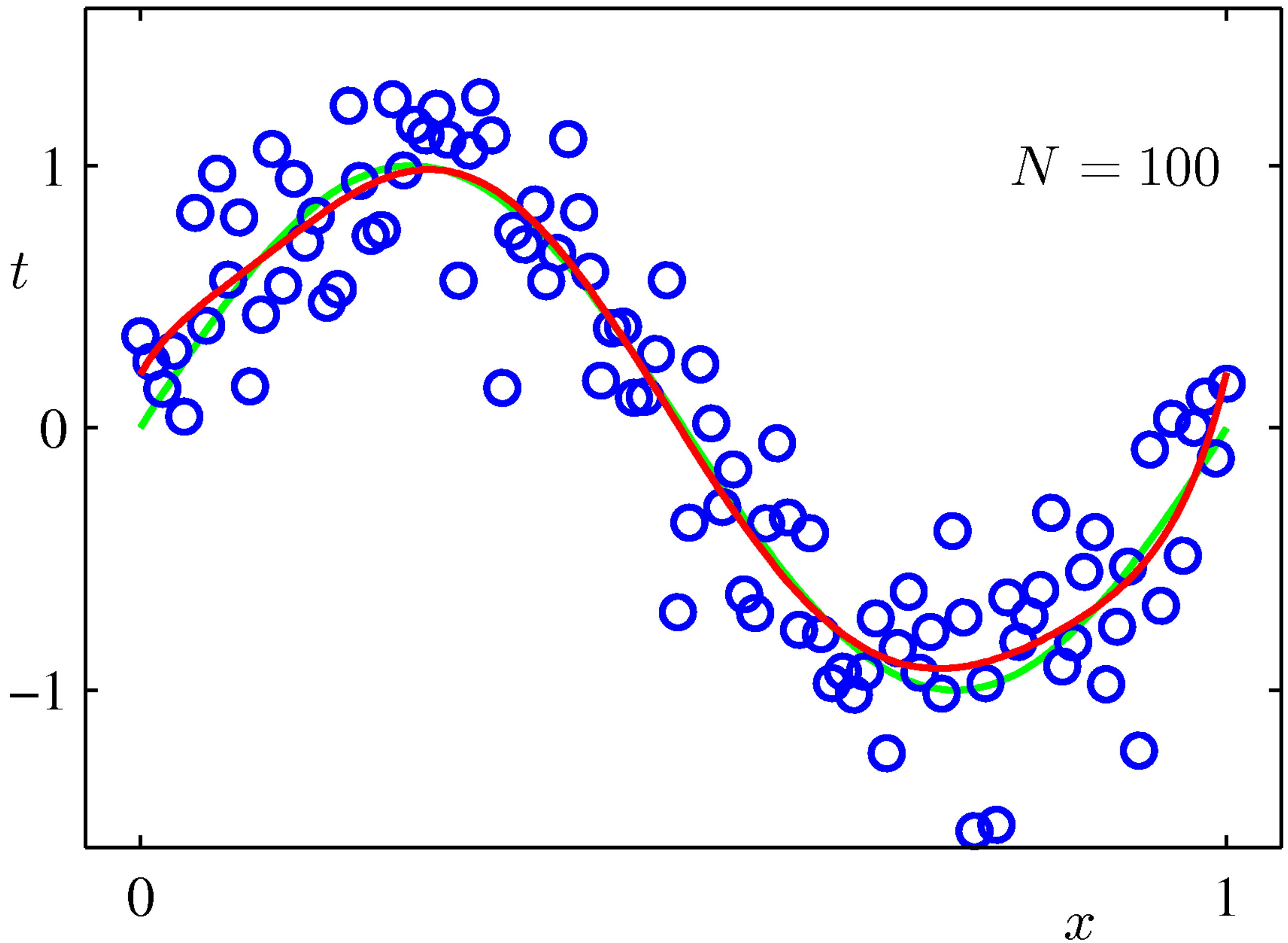
Effect of dataset size

- Polynomial of order 9 and $N = 15$



Effect of dataset size

- Polynomial of order 9 and $N = 100$



Regularization

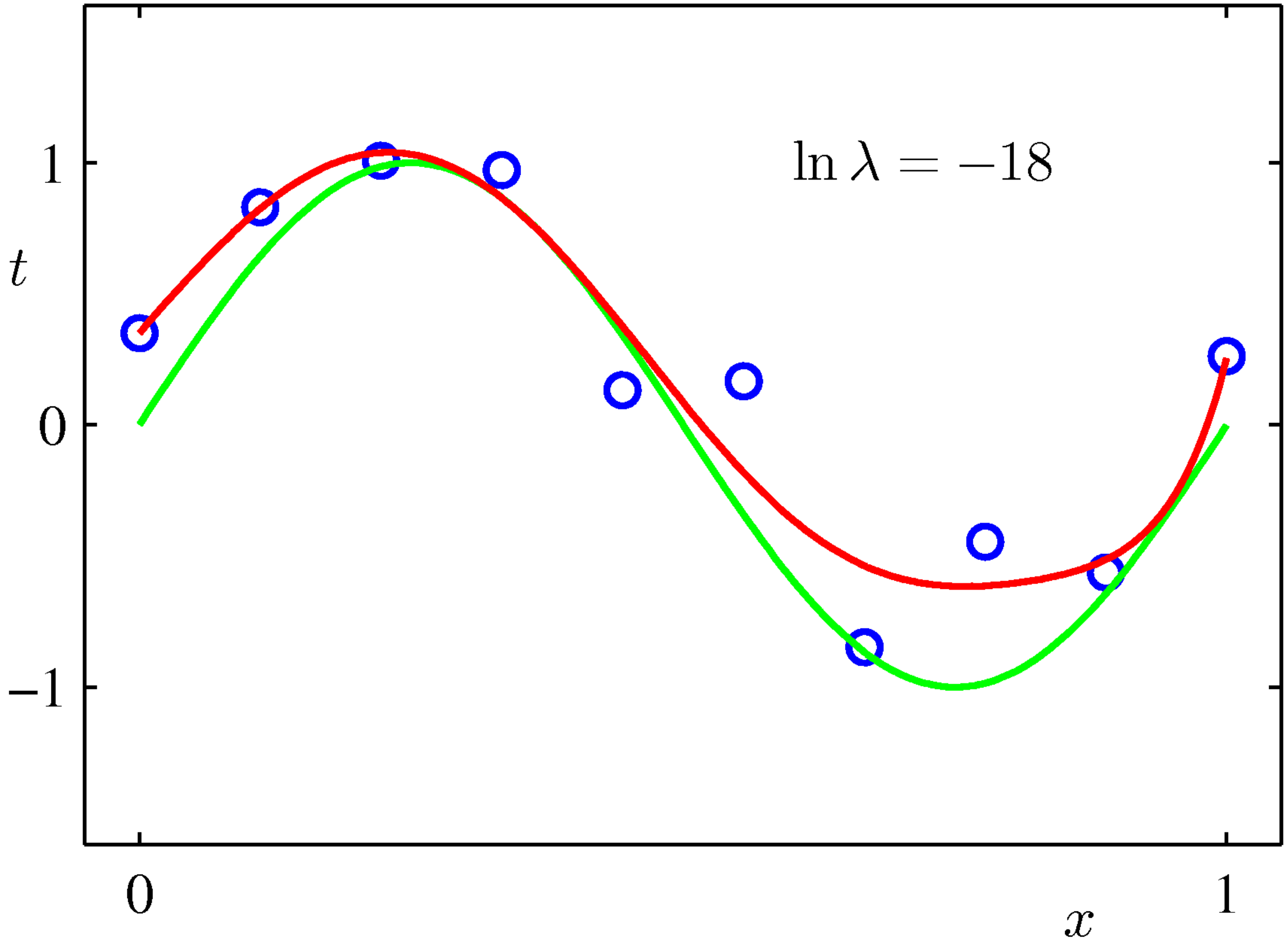
- Penalize large coefficients values

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

- λ becomes a model parameter

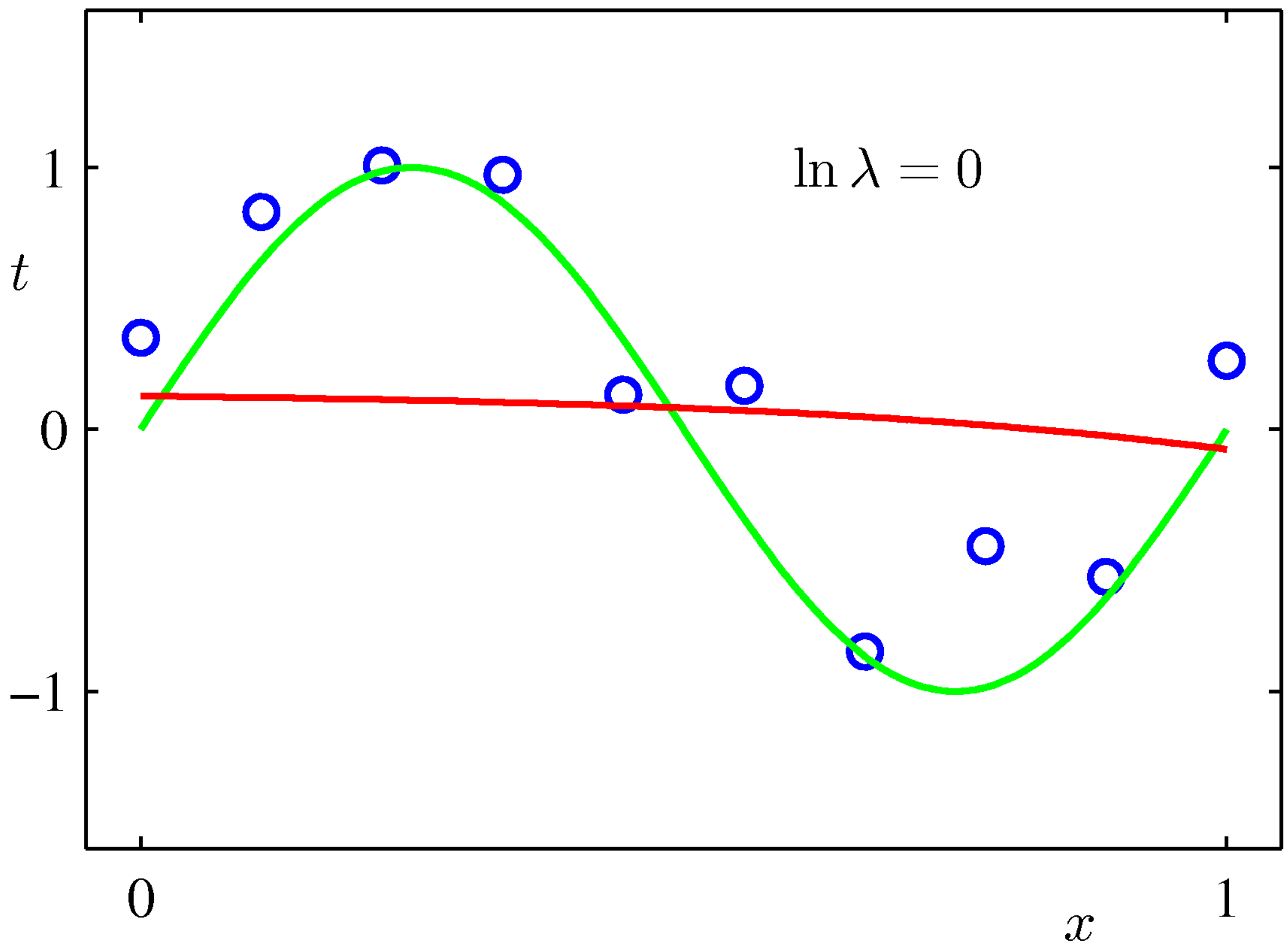
Regularization

- Regularization with $\ln \lambda = -18$



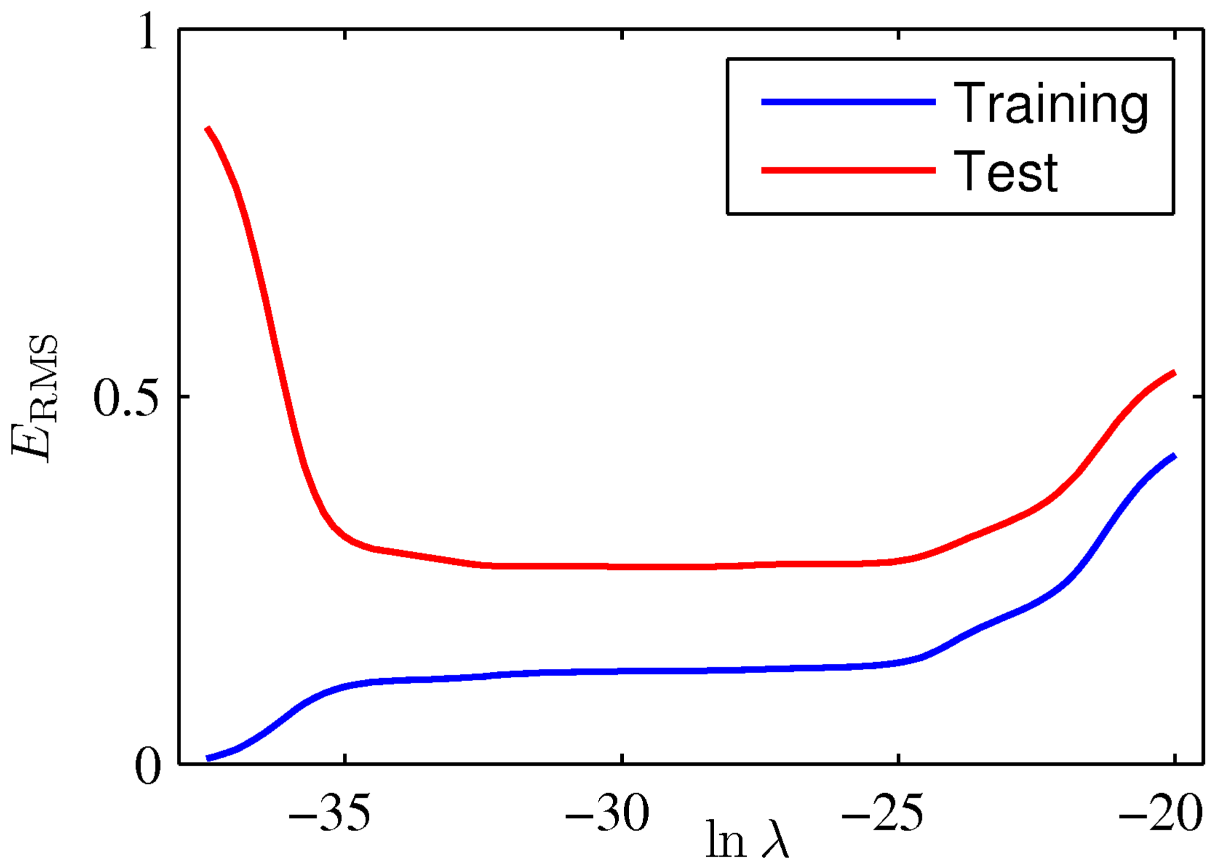
Regularization

- Regularization with $\ln \lambda = 0$



Regularization

- E_{RMS} versus $\ln \lambda$



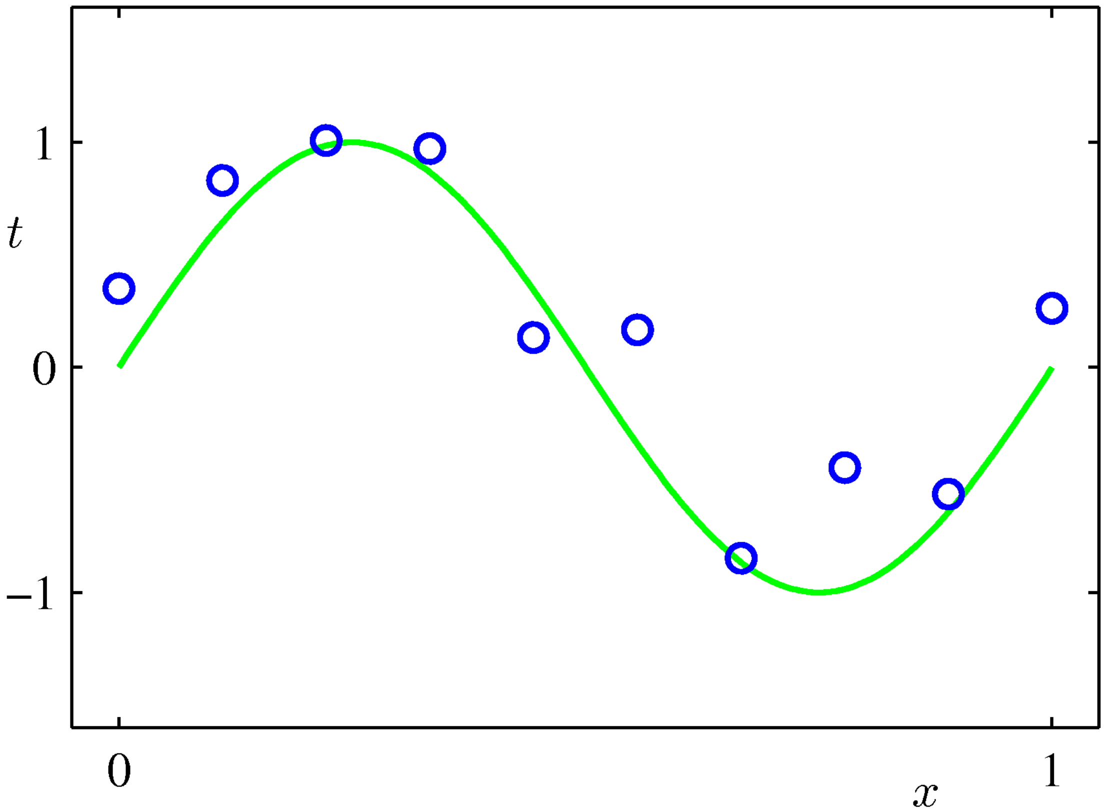
Regularization

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	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

A deeper analysis

Advanced Machine Learning

What is the issue?



$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} + \cdots$$

Linear basis function models

- General model is

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \varphi_j(\mathbf{x}) = \mathbf{w}^\top \varphi(\mathbf{x})$$

- φ_j are known are basis functions
- Typically, $\varphi_0(\mathbf{x}) = 1$ so that w_0 acts as bias

Linear basis function models

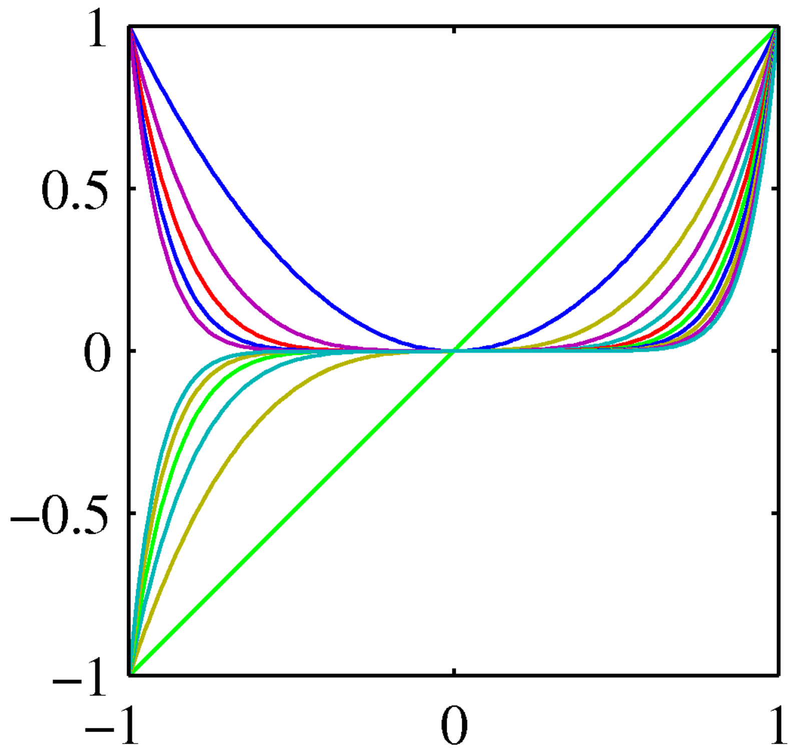
- General model is

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \varphi_j(\mathbf{x}) = \mathbf{w}^\top \varphi(\mathbf{x})$$

- Polynomial basis functions:

  $\varphi_j(\mathbf{x}) = x^j$

- These are global functions



Linear basis function models

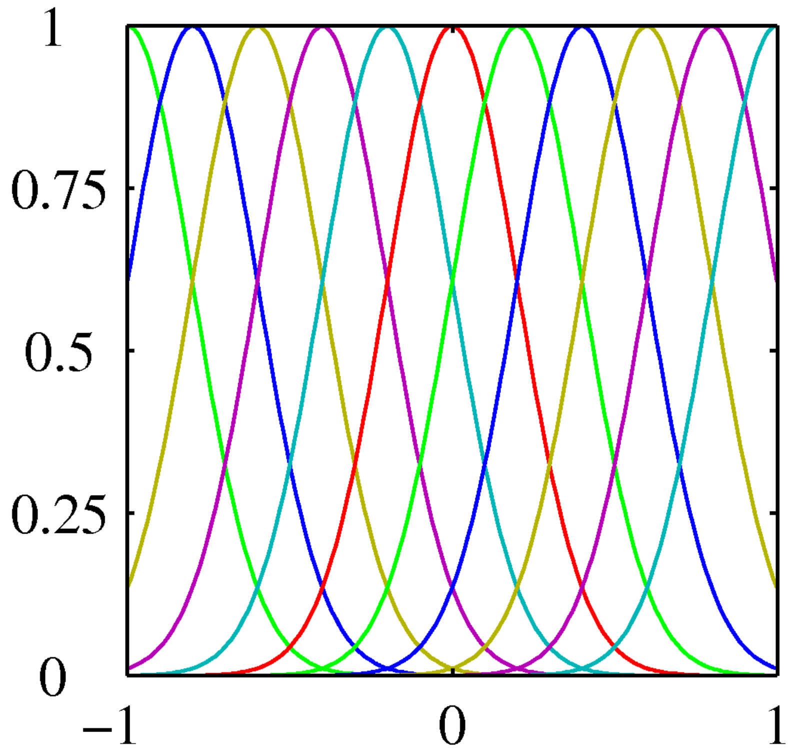
- General model is

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \varphi_j(\mathbf{x}) = \mathbf{w}^\top \varphi(\mathbf{x})$$

- Gaussian basis functions:

$$\varphi_j(\mathbf{x}) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$

- These are local functions
  - > μ_j controls location
  - > s controls scale



Linear basis function models

- General model is

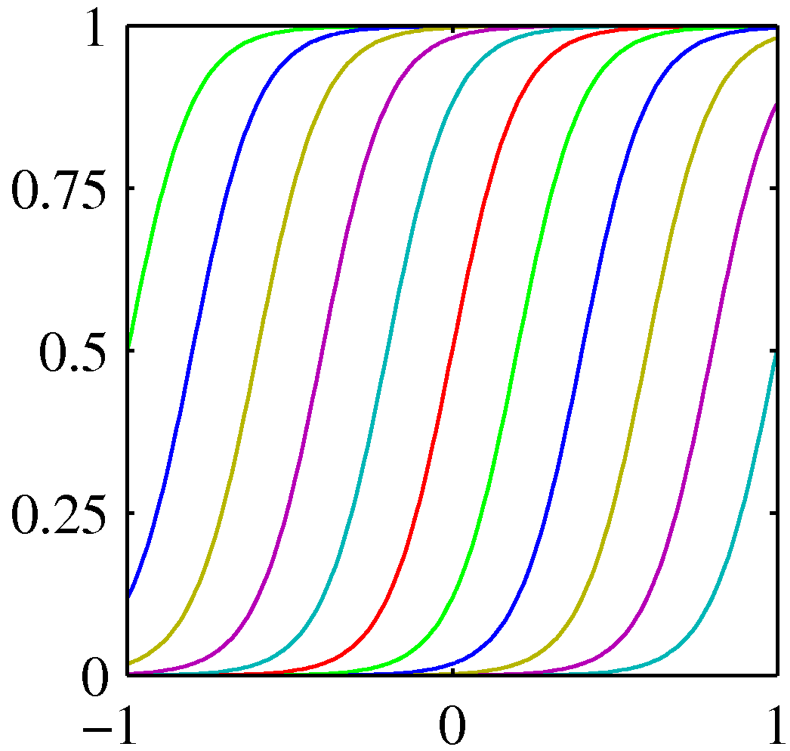
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \varphi_j(\mathbf{x}) = \mathbf{w}^\top \varphi(\mathbf{x})$$

- Sigmoidal basis functions:

$$\varphi_j(\mathbf{x}) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

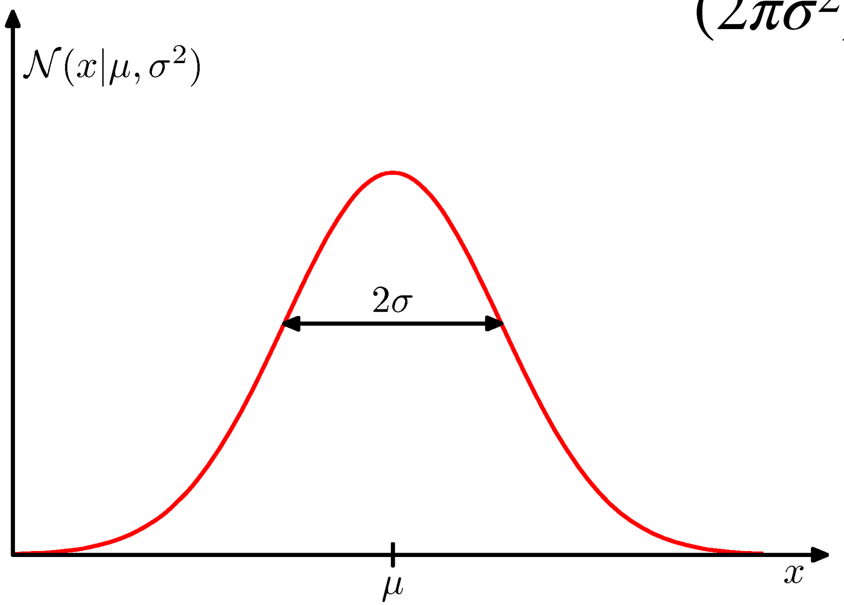


Maximum likelihood

- Assume observations from a deterministic function with added Gaussian noise:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon \quad \text{where} \quad p(\epsilon \,|\, \beta) = \mathcal{N}(\epsilon \,|\, 0, \beta^{-1})$$

- Note that $\mathcal{N}(x \,|\, \mu, \sigma^2) = \dfrac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{ -\dfrac{1}{2\sigma^2}(x-\mu)^2 \right\}$



$$\beta = 1/\sigma^2$$

$$\mathcal{N}(x \,|\, \mu, \sigma^2) > 0$$

$$\int_{-\infty}^{\infty} \mathcal{N}(x \,|\, \mu, \sigma^2)\, \mathrm{d}x = 1$$

Maximum likelihood

- Assume observations from a deterministic function with added Gaussian noise:

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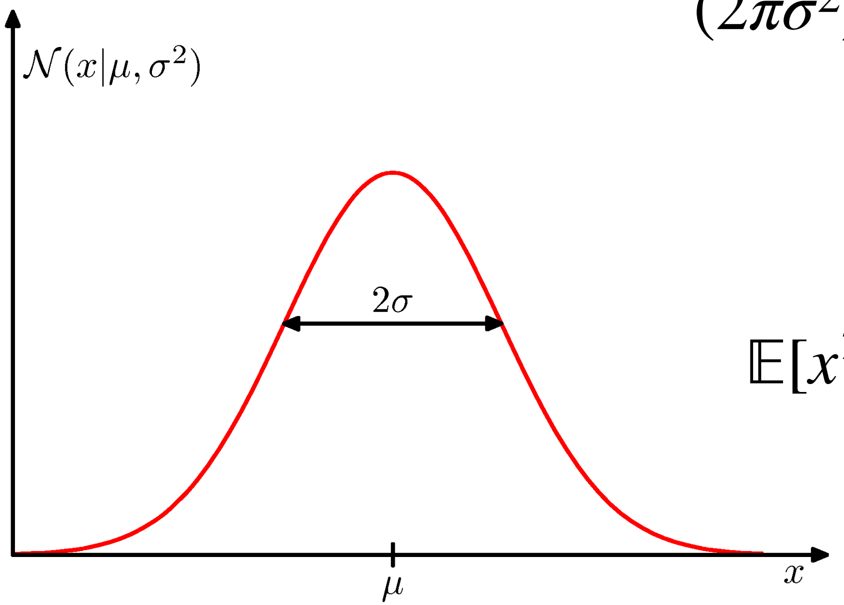


$$\mathbb{E}[x] = \int_{-\infty}^{\infty} x\mathcal{N}(x \,|\, \mu, \sigma^2)\,\mathrm{d}x = \mu$$

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} x^2\mathcal{N}(x \,|\, \mu, \sigma^2)\,\mathrm{d}x = \mu^2 + \sigma^2$$

$$\mathrm{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$

Maximum likelihood

- Assume observations from a deterministic function with added Gaussian noise:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon \quad \text{where} \quad p(\epsilon \mid \beta) = \mathcal{N}(\epsilon \mid 0, \beta^{-1})$$

- This is the same as saying

$$p(t \mid \mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

- Recall: $y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \varphi_j(\mathbf{x}) = \mathbf{w}^\top \varphi(\mathbf{x})$

Maximum likelihood

- This is the same as saying

$$p(t \mid \mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(\mathbf{x}, \mathbf{w}), \beta^{-1})$$

- Given observed inputs $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and targets $\mathbf{t} = [t_1, \ldots, t_N]^\top$, we obtain the likelihood function:

$$p(\mathbf{t} \mid \mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid \mathbf{w}^\top \varphi(\mathbf{x}_n), \beta^{-1})$$

Maximum likelihood

- Taking the logarithm, we get

$$\ln p(\mathbf{t} \,|\, \mathbf{w}, \beta) = \sum_{n=1}^{N} \ln \mathcal{N}(t_n \,|\, \mathbf{w}^\top \varphi(\mathbf{x}_n), \beta^{-1})$$

$$= \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w})$$

where $E_D(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{t_n - \mathbf{w}^\top \varphi(\mathbf{x}_n)\}^2$

- Recall: $\mathcal{N}(x \,|\, \mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{ -\frac{1}{2\sigma^2}(x-\mu)^2 \right\}$

Maximum likelihood

- Computing the gradient and setting it to zero yields

$$\nabla_{\mathbf{w}} \ln p(\mathbf{t} \mid \mathbf{w}, \beta) = \beta \sum_{n=1}^{N} \{t_n - \mathbf{w}^\top \varphi(\mathbf{x}_n)\} \varphi(\mathbf{x}_n)^\top = 0$$

- Solve for $\mathbf{w}$, we get

The Moore-Penrose pseudo-inverse

$$\mathbf{w}_{\mathrm{ML}} = \left(\boldsymbol{\Phi}^\top \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^\top \mathbf{t}$$

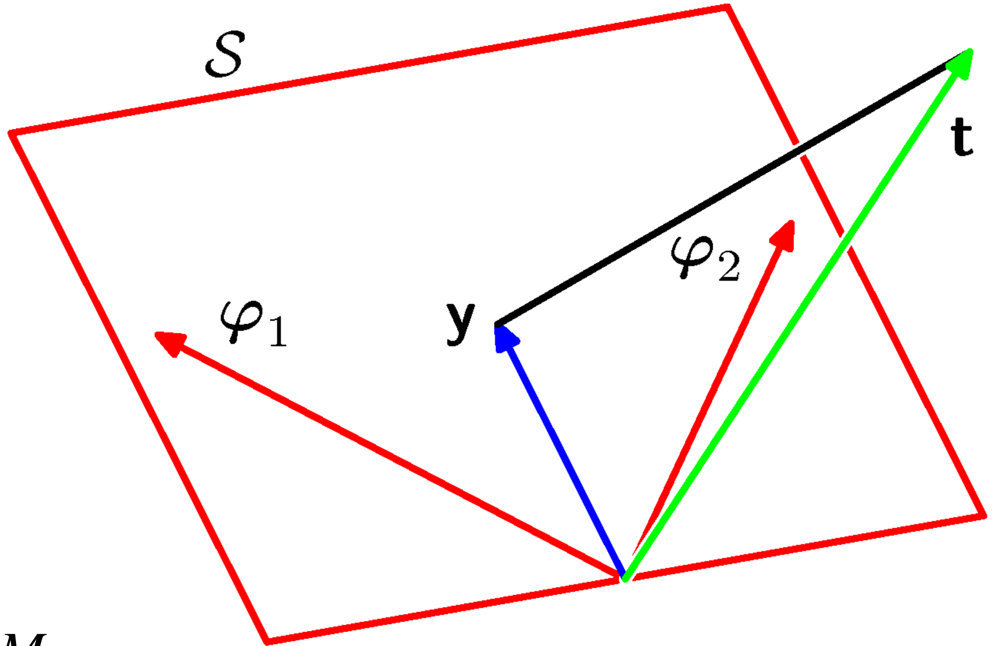
with

$$\boldsymbol{\Phi} = \begin{pmatrix} \varphi_0(\mathbf{x}_1) & \varphi_1(\mathbf{x}_1) & \cdots & \varphi_{M-1}(\mathbf{x}_1) \\ \varphi_0(\mathbf{x}_2) & \varphi_1(\mathbf{x}_2) & \cdots & \varphi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_0(\mathbf{x}_N) & \varphi_1(\mathbf{x}_N) & \cdots & \varphi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

Interpretation

- Consider $\mathbf{y} = \mathbf{\Phi}\mathbf{w}_{\text{ML}} = [\varphi_1, \ldots, \varphi_M]\mathbf{w}_{\text{ML}}$

$$\underbrace{\mathbf{y} \in \mathscr{S}}_{M\text{-dimensional}} \subseteq \underbrace{\mathscr{T}}_{N\text{-dimensional}}$$



- $\mathscr{S}$ is spanned by $\varphi_1, \ldots, \varphi_M$
- $\mathbf{w}_{\text{ML}}$ minimizes the distance between $\mathbf{t}$ and its orthogonal projection on $\mathscr{S}$, i.e., $\mathbf{y}$

Regularization

- Consider the error function

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

data term + regularization term

- With the sum-of-squares error function and a quadratic regularizer, we get

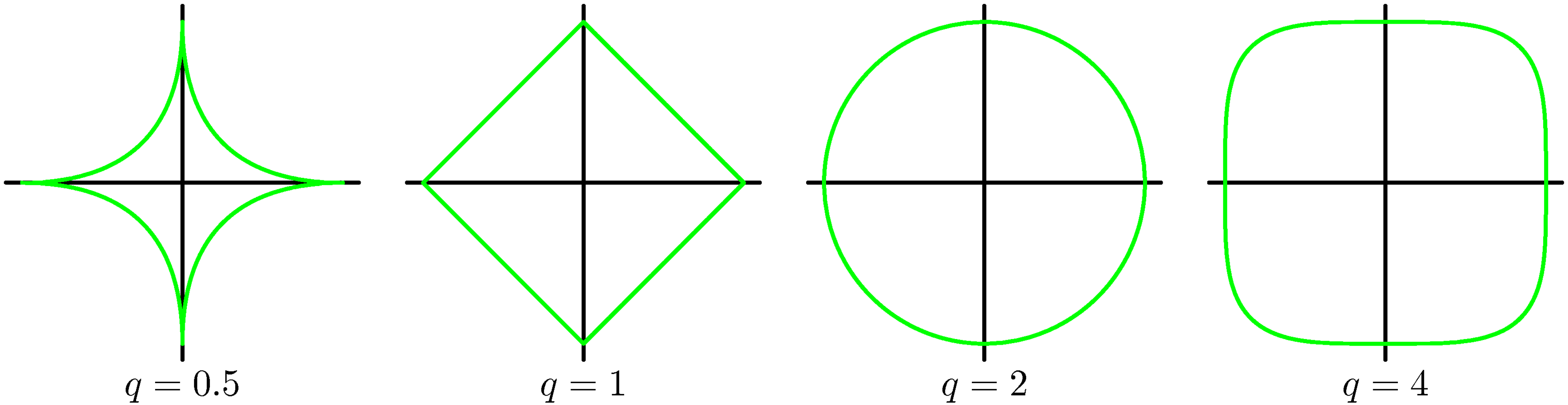
$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^\top \varphi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$$

- This is minimized by $\mathbf{w} = \left(\lambda\mathbf{I} + \boldsymbol{\Phi}^\top\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^\top\mathbf{t}$

Regularization

- With a more general regularizer, we have

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^\top \varphi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$



lasso quadratic

Regularization

- Lasso tends to generate sparser solutions than a quadratic regularizer