Overfitting, Regularization, Cross-validation

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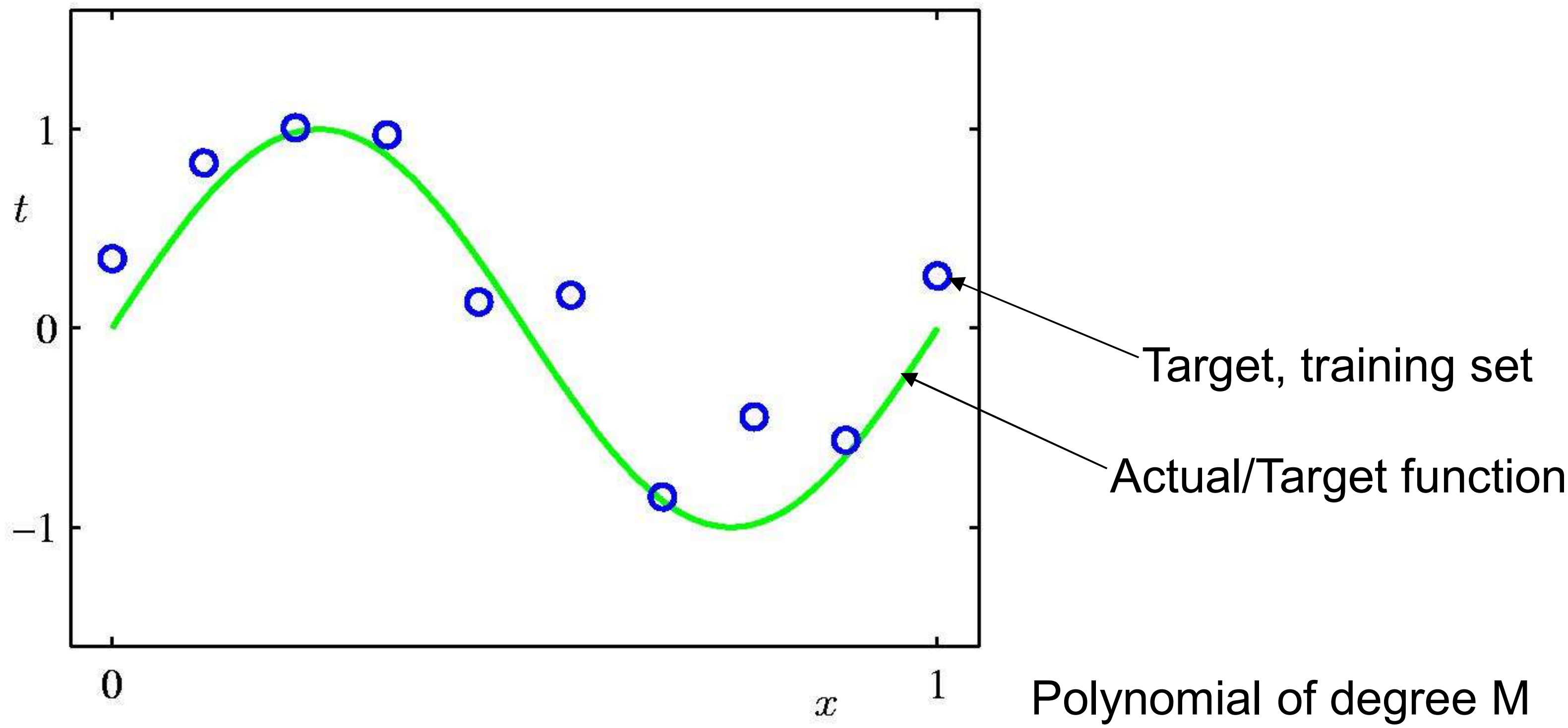
Overfitting, Regularization, Cross-validation

1. Overfitting: model learns “small details” of the training set and is unable to correctly classify cases of the test set (usually: too many parameters/degrees of freedom)
2. Regularization: preventing overfitting by imposing some constraints on values or the number of model parameters
3. Cross-validation: monitoring the error both on the training and the test set

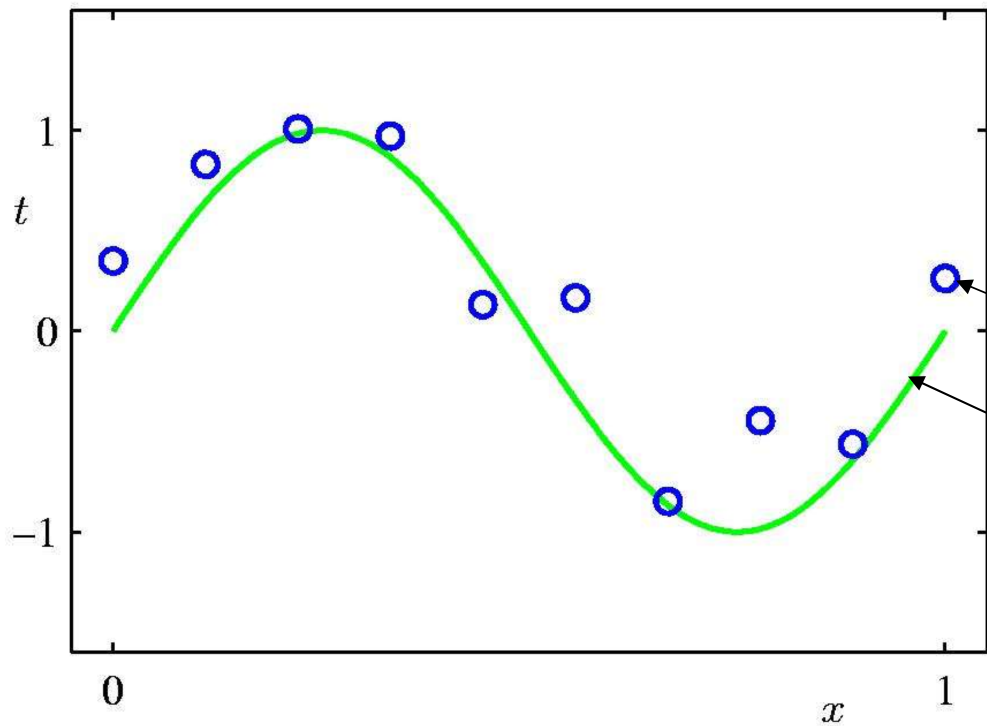
Regression: Polynomial Curve Fitting



Polynomial of degree M

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

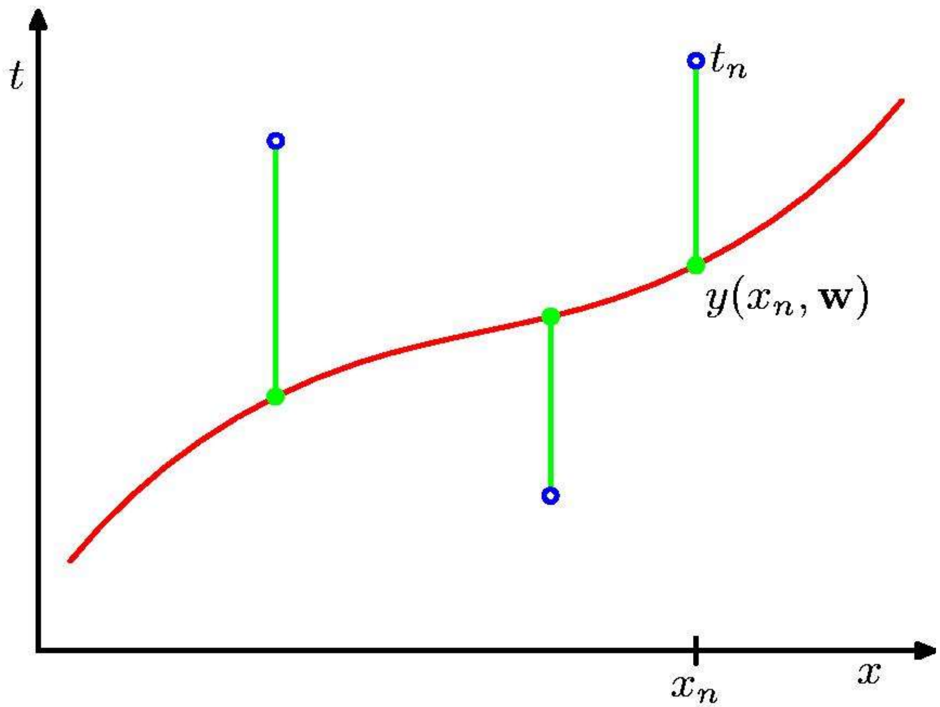
Regression: Polynomial Curve Fitting



Polynomial of degree M

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

Sum-of-Squares Error Function



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

Through optimization,
we need to find the model (red)
y(x,w) that minimizes the
error function.

E_{SSE}(w): Sum squared error: 2E(w)

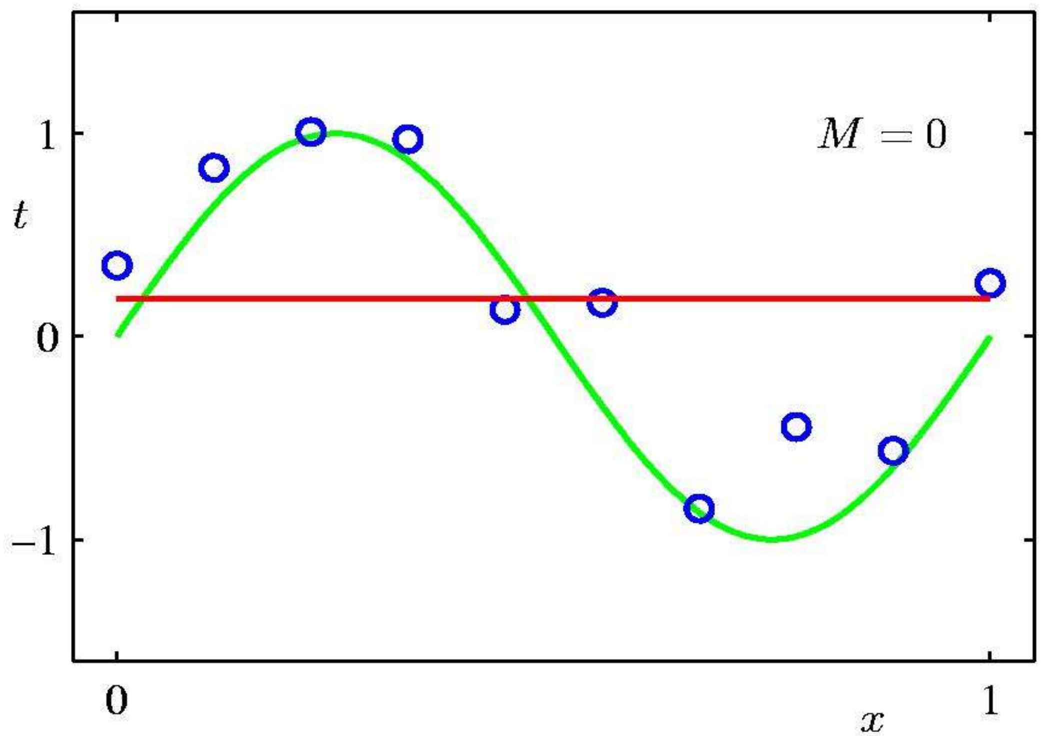
E_{RMS}(w): Root mean squared error

$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$$

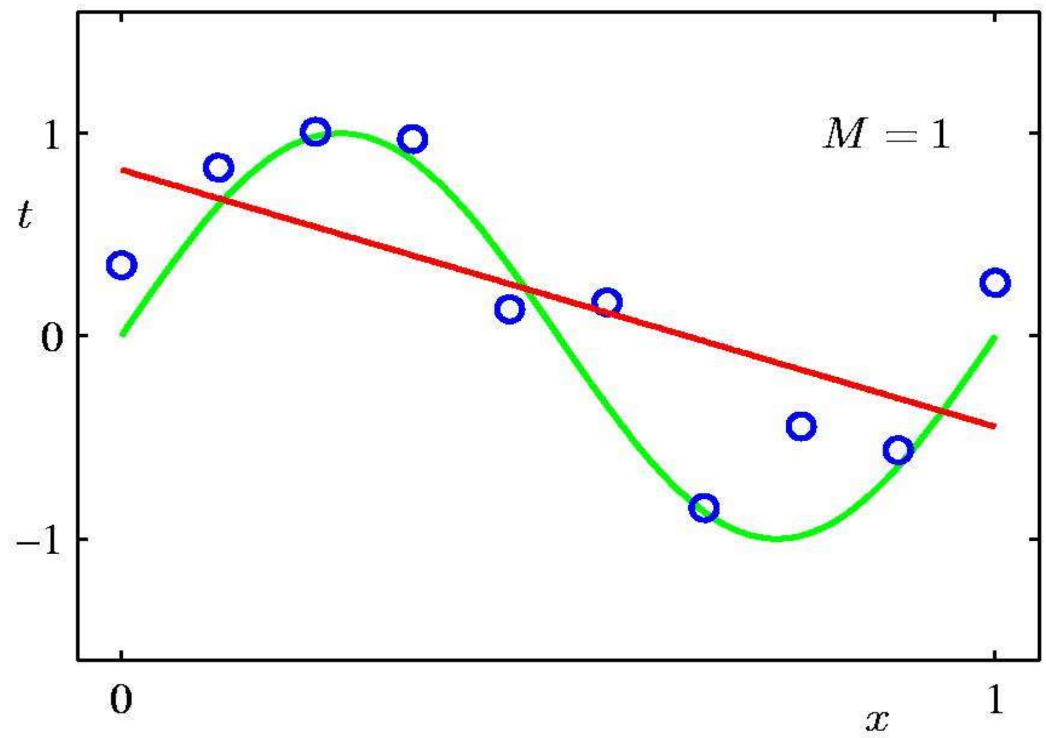
Finding optimal coefficients:
the ***polyfit.m*** function.

|x-y| instead of (x-y)2?
Then error wouldn't be "smooth"…

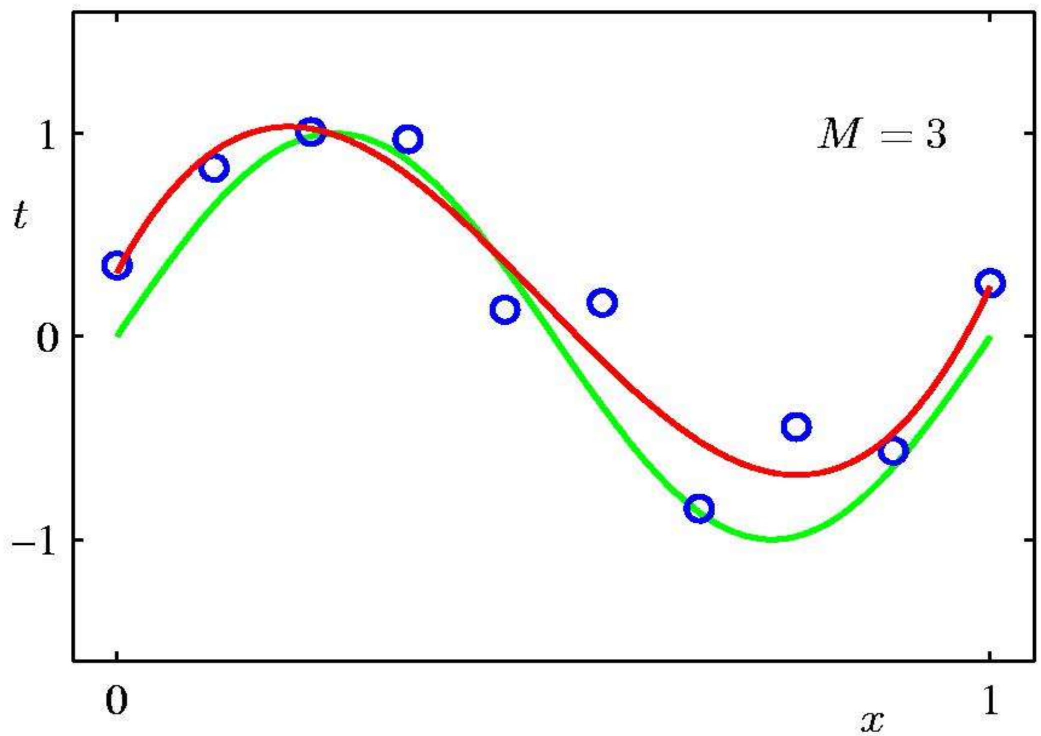
0^{th} Order Polynomial



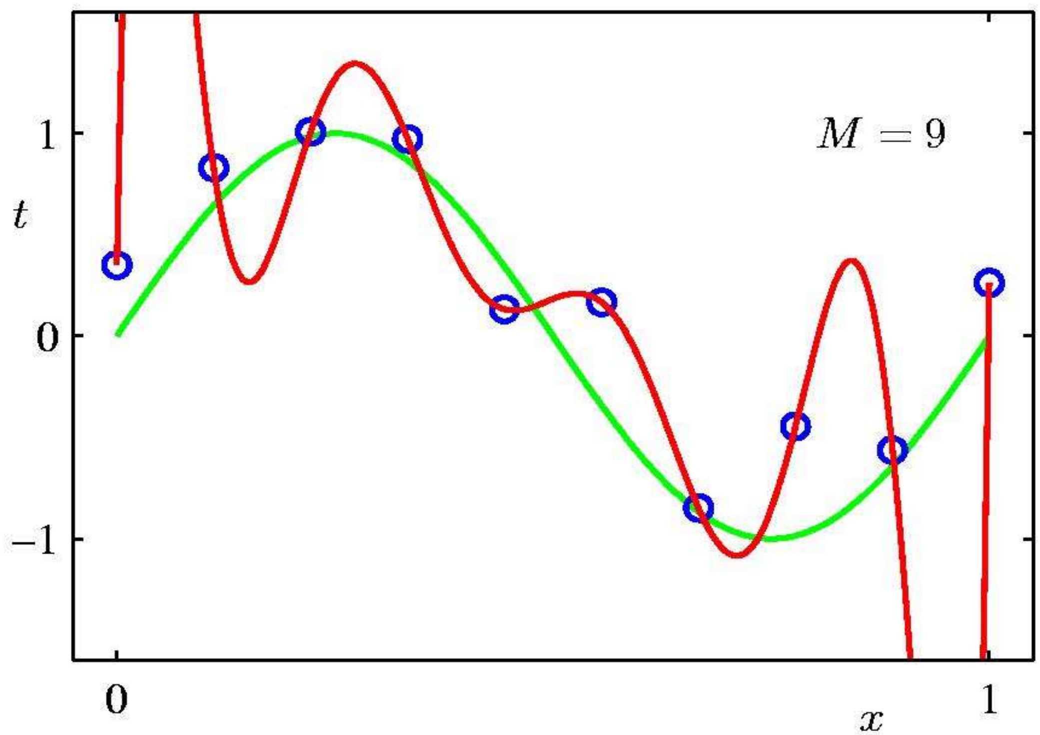
1^{st} Order Polynomial



3^{rd} Order Polynomial



9th Order Polynomial (over-fitting)



Polynomial Coefficients

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	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

REGULARIZATION

Regularization is a powerful technique of limiting overfitting.

The key idea: somehow enforce the absolute values of model parameters to be relatively small (in our case: coefficients of the polynomial).

For example: add to the error function an extra term: "the sum of squared coefficients of your model":

$$\lambda \sum_{i=0}^{M} w_i^2$$

where λ a tunable parameter that controls the size "punishment" for too big values of coefficients.

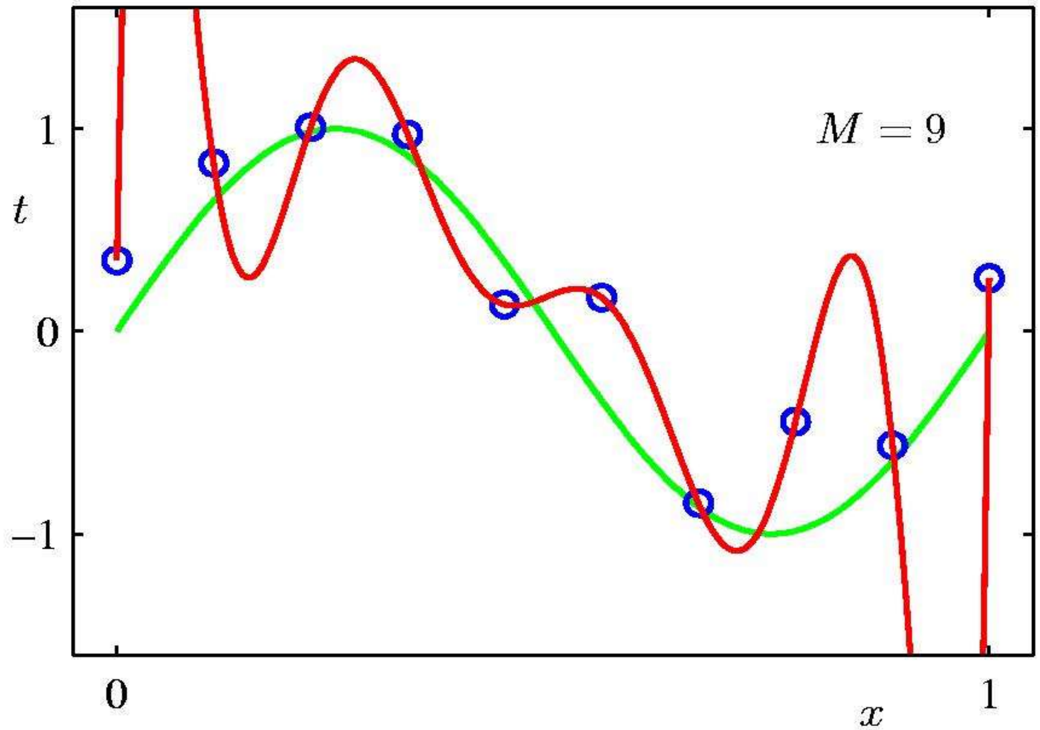
Regularization

- **Penalize large coefficient values**

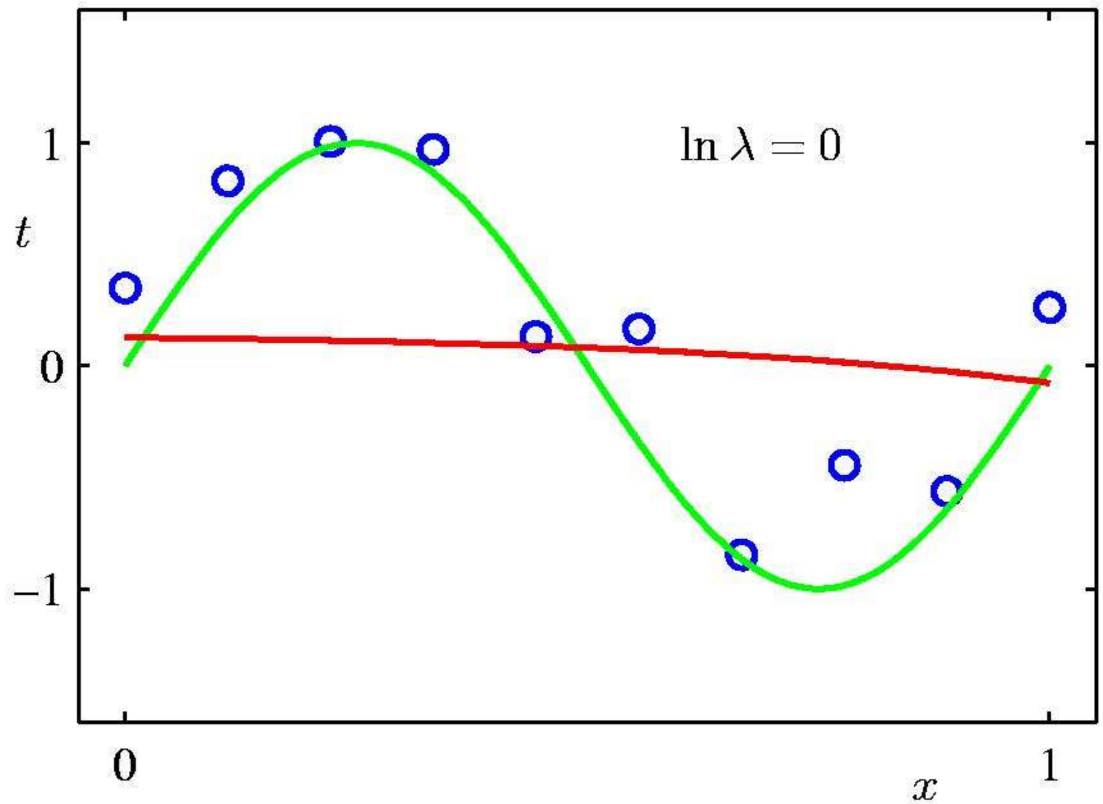
$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

- **Minimize training error while keeping the weights small. This is known as:**
    - shrinkage,
    - ridge regression,
    - weight decay (neural networks)

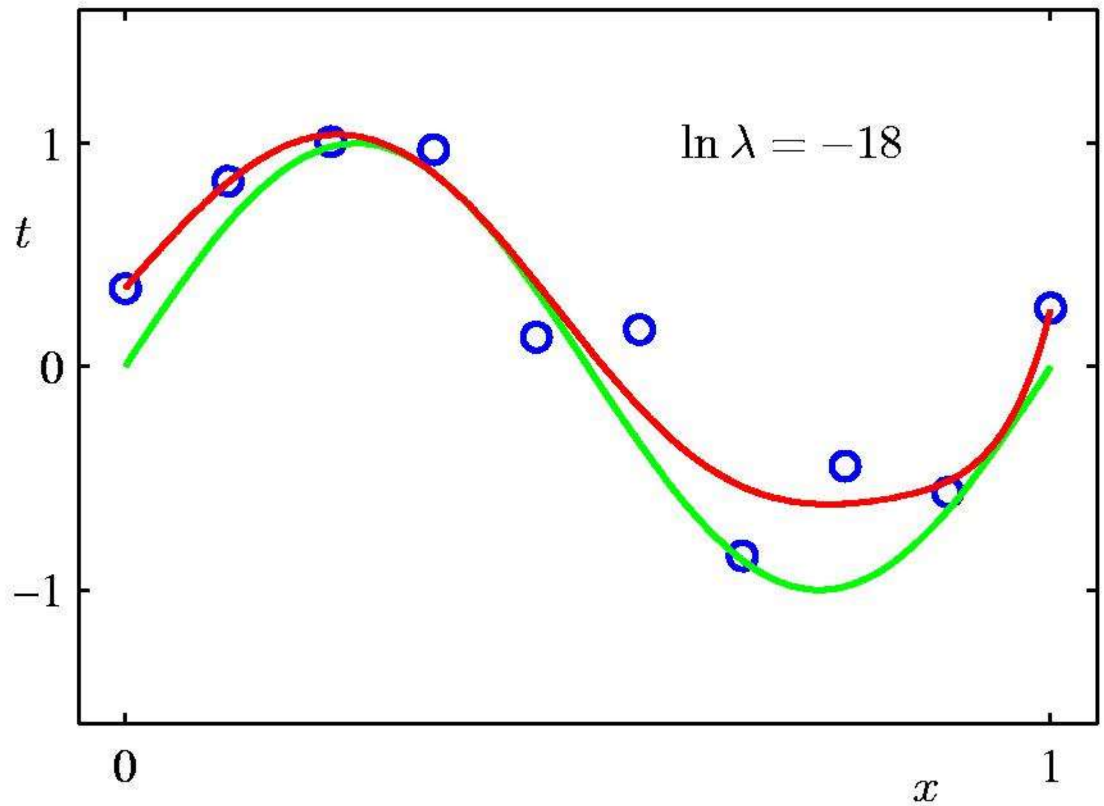
Regularization (M=9; λ=0)



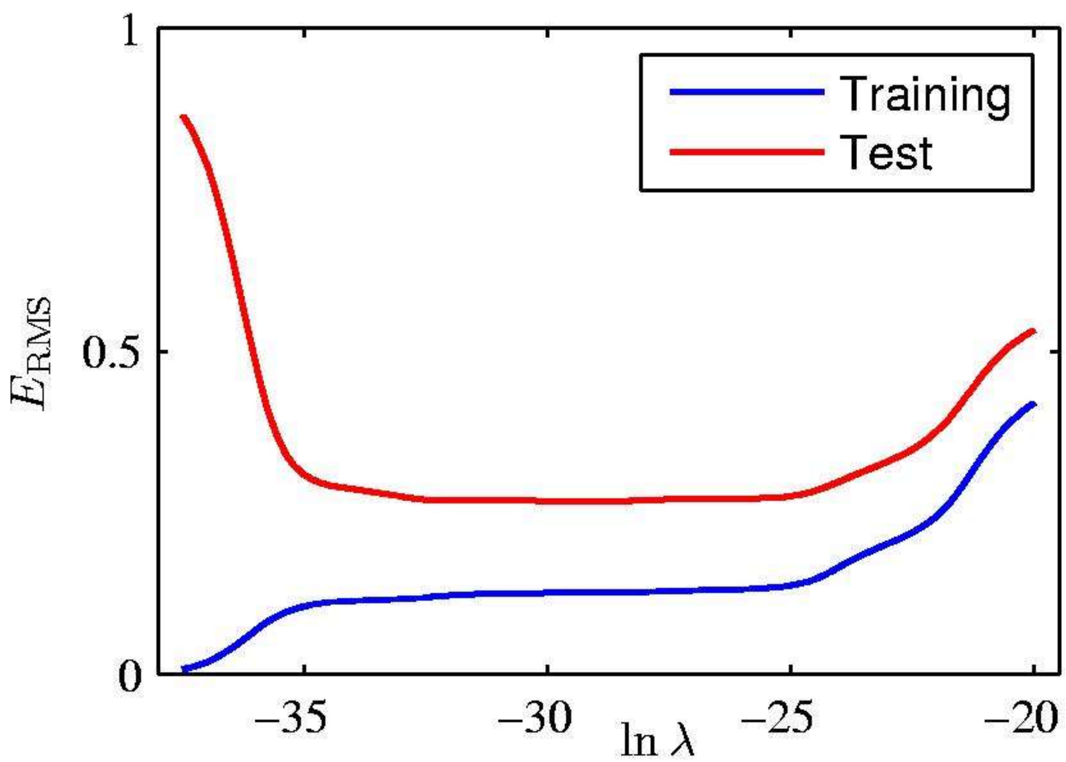
Regularization (d=9; λ=1)



Regularization (M=9; λ=1.5230e-08)



Regularization: error vs. lambda



Polynomial Coefficients

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