Linear Models of Regression

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Regression

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- Need to define a loss function for optimizing model parameters $\mathbf{w}$

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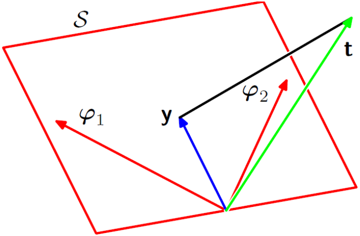
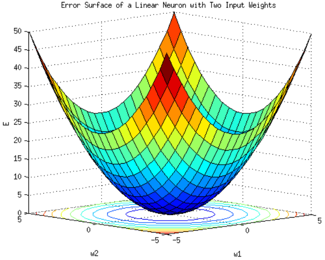
- Equating derivative w.r.t **w** to 0

$$\nabla_\mathbf{w} J(\mathbf{w}) = \nabla_\mathbf{y} J(\mathbf{w})\ \nabla_\mathbf{w}\mathbf{y}$$
$$= \mathbf{X}^\mathsf{T}(\mathbf{t} - \mathbf{X}\mathbf{w}) = \mathbf{0}$$

$$\boxed{\mathbf{w} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{t}}$$

Geometric Interpretation of Least Squares





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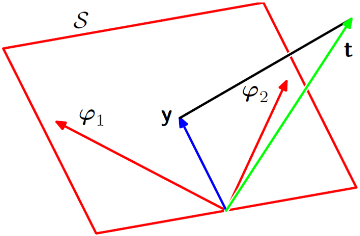

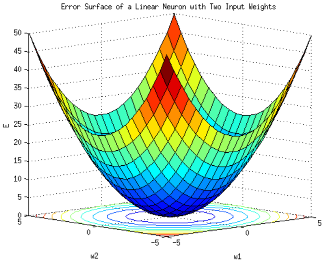

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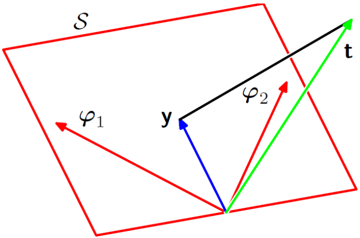

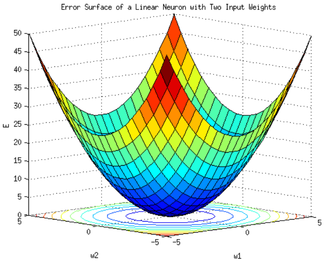

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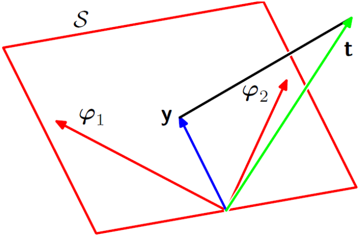

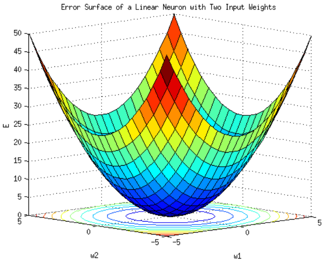

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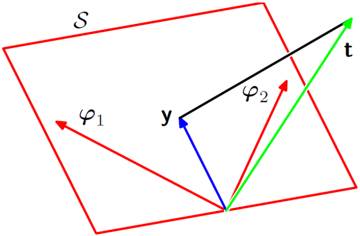

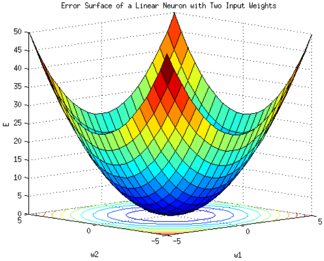

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- For the LS optimality criterion

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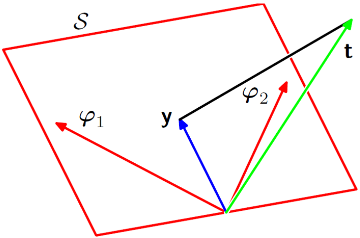

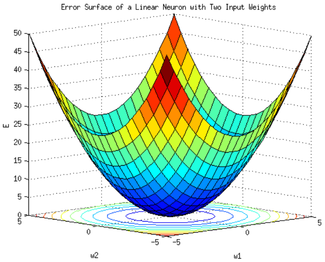

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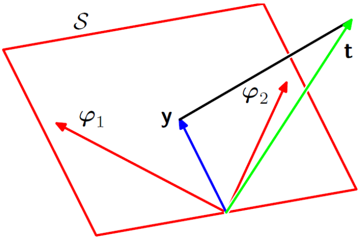

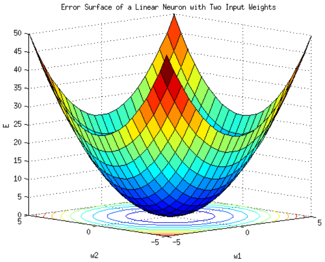

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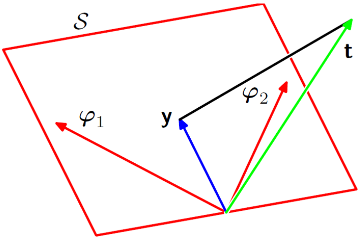

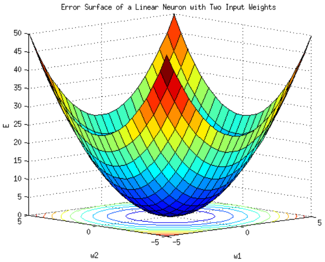

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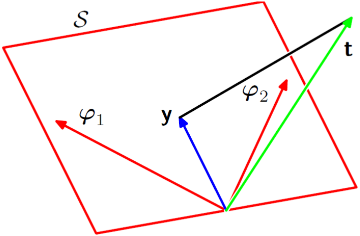

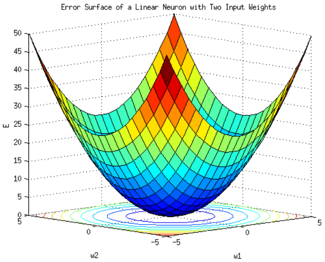

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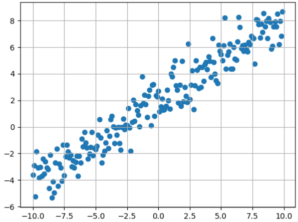
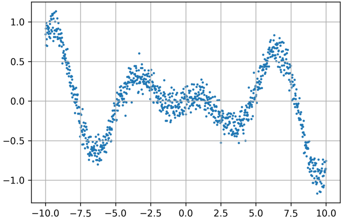
  - Also referred to as pseudo inverse sol.

Nonlinear Input-Output Relations



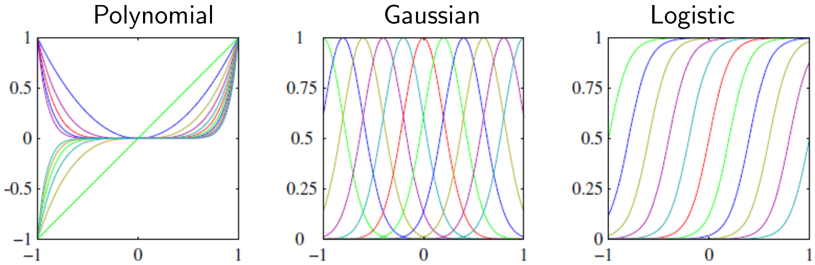


- Polynomial curve fitting can be used to model ninlinear i/o relation

$$\hat{t} = y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M$$
$$= \mathbf{w}^{\mathsf{T}} \phi(\mathbf{x}) \qquad \text{(Model is linear in } \mathbf{w}\text{)}$$

- $\phi(.) : \mathbb{R}^1 \rightarrow \mathbb{R}^M$ - nonlinear transformation to higher dim. space

Kernel Examples



Kernel Examples

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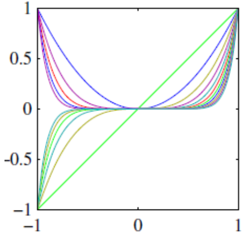
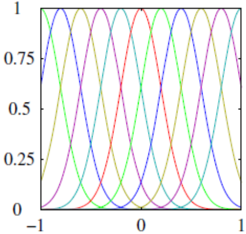


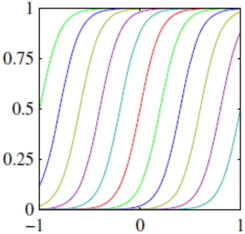
$\phi_j(x) = x^j$

Gaussian



$\phi_j(x) = \exp\left(-\frac{x-\mu_j}{2\sigma^2}\right)$

Logistic



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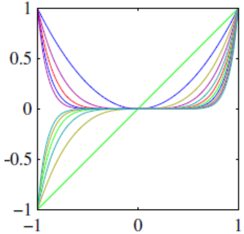

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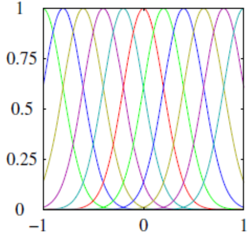

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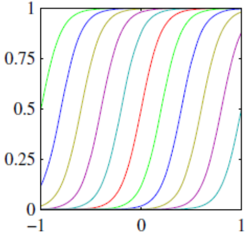

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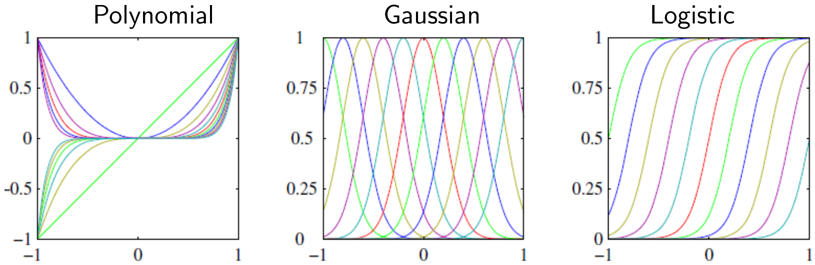

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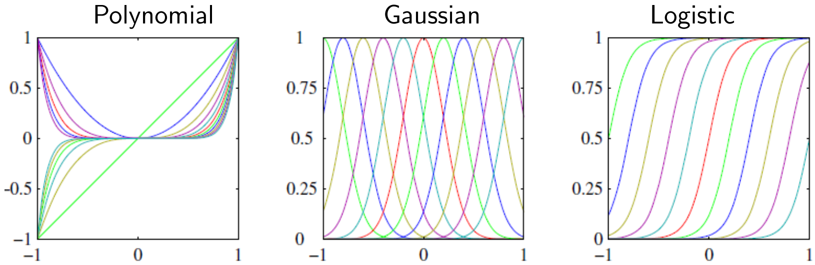

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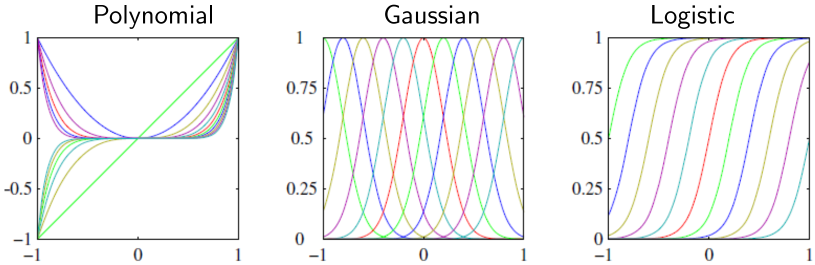

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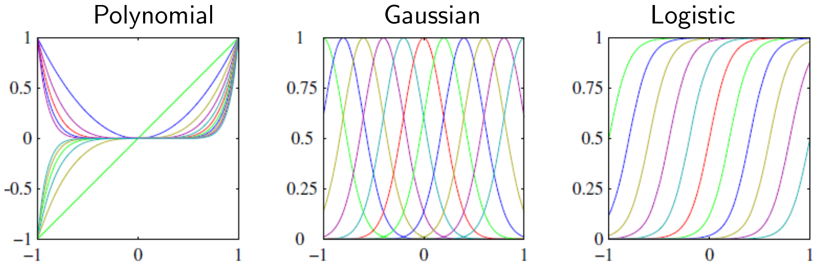

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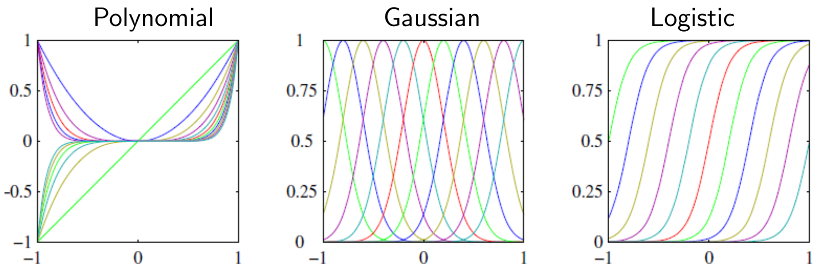

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  - Local kernels are preferable for functions with varying characteristics

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- $\mathbf{x}_n = [x_{n1} \ x_{n2}]^\mathsf{T} \in \mathbb{R}^2$ can be mapped using 2^{nd} order polynomial kernel as $\phi(\mathbf{x}_n) = [1 \ x_{n1} \ x_{n2} \ x_{n1}^2 \ x_{n2}^2 \ x_{n1}x_{n2}]^\mathsf{T} \in \mathbb{R}^6$

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- The target t_n is regressed from the kernel representation $\phi(\mathbf{x}_n)$ as

$$\hat{t}_n = \mathbf{w}^\mathsf{T}\phi(\mathbf{x}_n) \qquad \mathbf{w} \in \mathbb{R}^M$$

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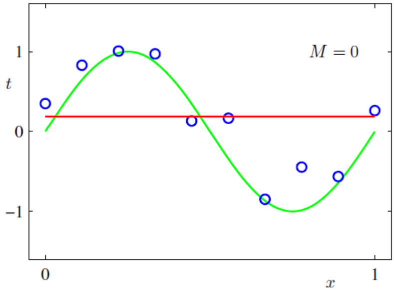
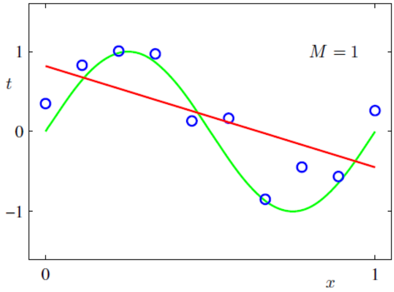
- The last layer of DNNs typically performs linear regression on $\phi(\mathbf{x}_n)$

Effect of Model Order M: $t = \sin(\pi x) + \epsilon$





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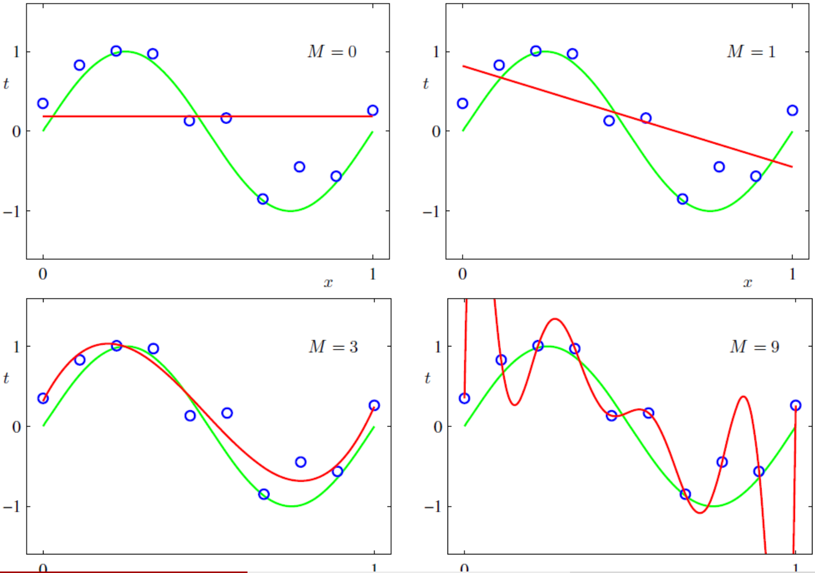

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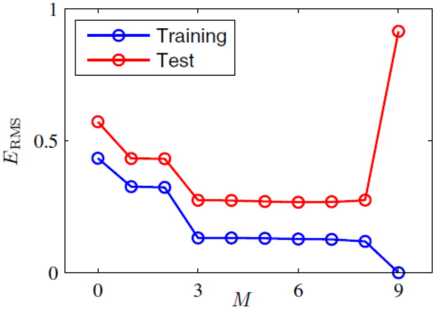

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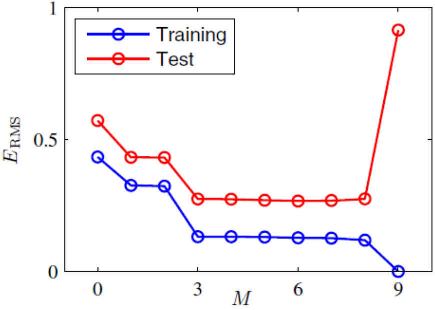

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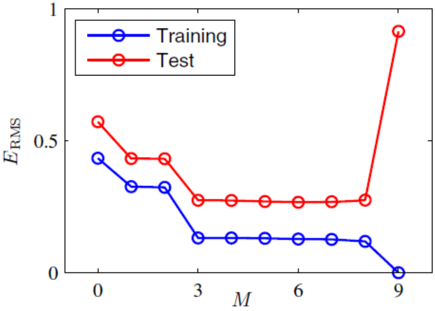

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$w_0^\star$	0.19	0.82	0.31	0.35
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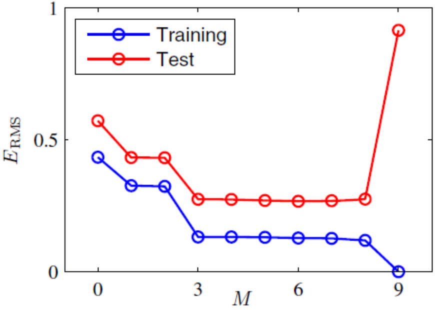

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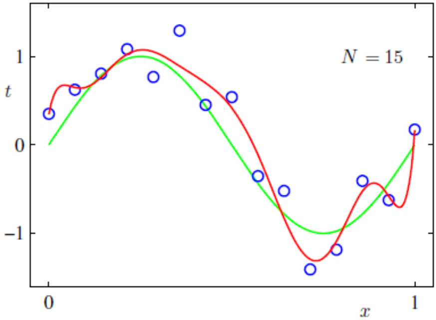
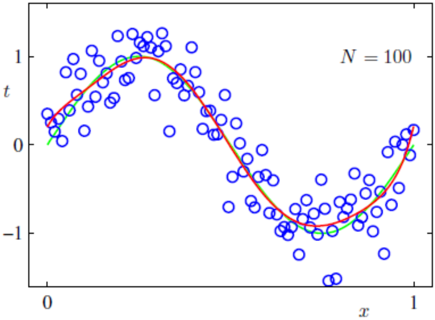
Amount of Training Data ($M = 9$)





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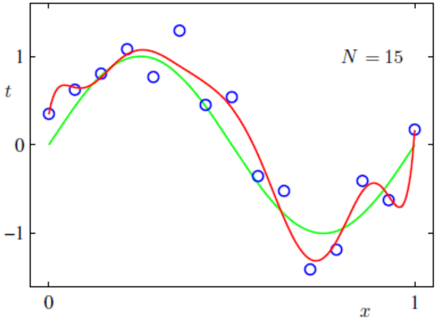

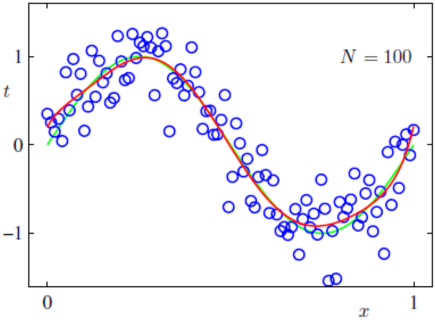

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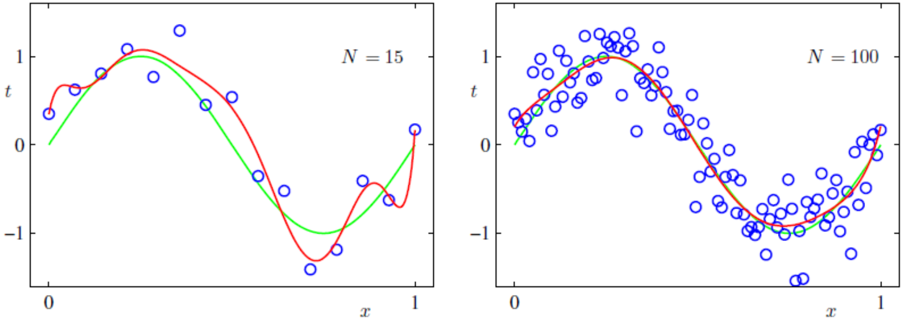

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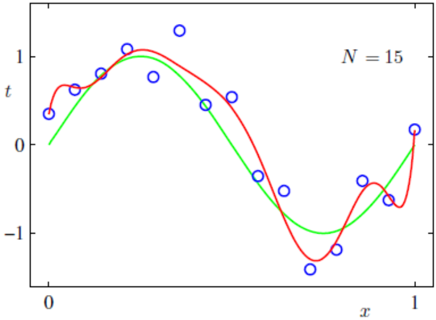

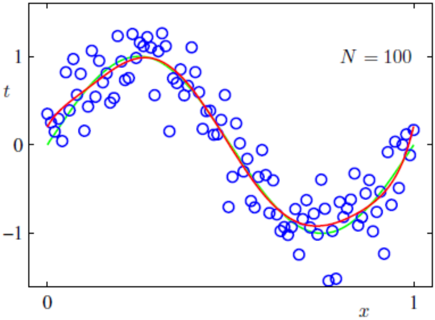

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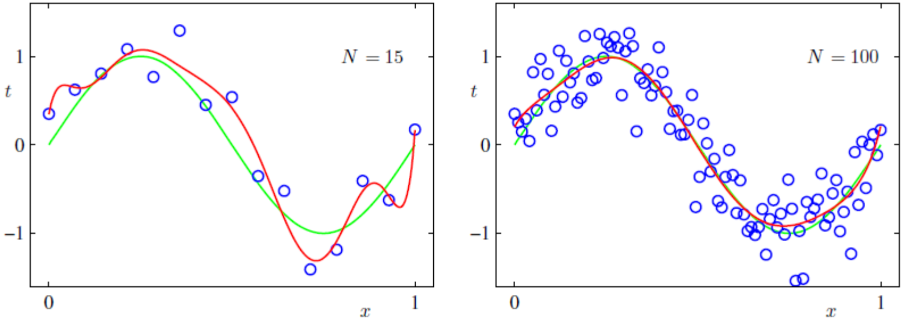

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- A way forward: arrest the growth of the model weights

Regularized Least Squares

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- Add a penalty term to the error term to discourage weight growth

$$J(\mathbf{w}) = \underbrace{E_D(\mathbf{w})}_{\text{Data Term}} + \underbrace{\lambda E_W(\mathbf{w})}_{\text{Regularization Term}}$$

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- Regularization term conditions the autocorrelation matrix!

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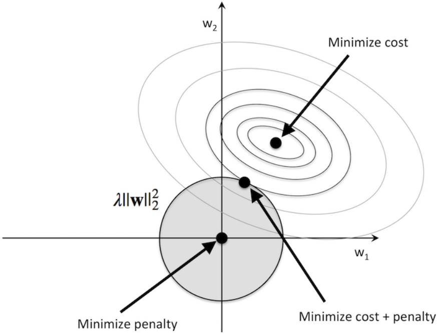

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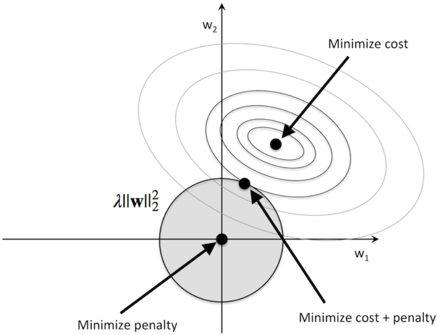
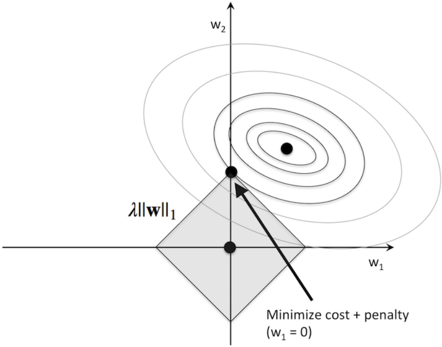
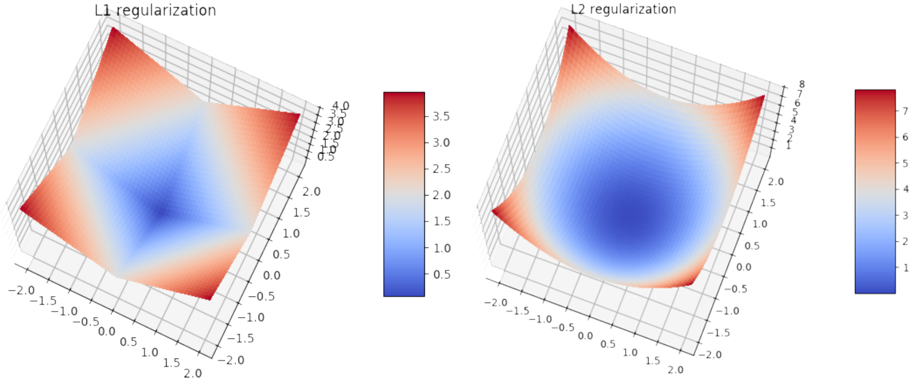


L_2 Regularizer



L_1 Regularizer

L_1 vs L_2



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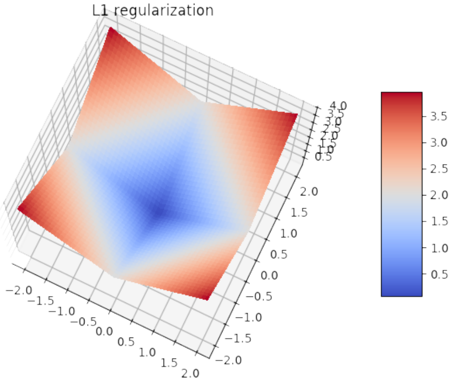

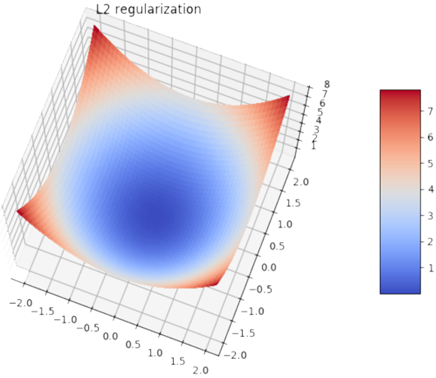

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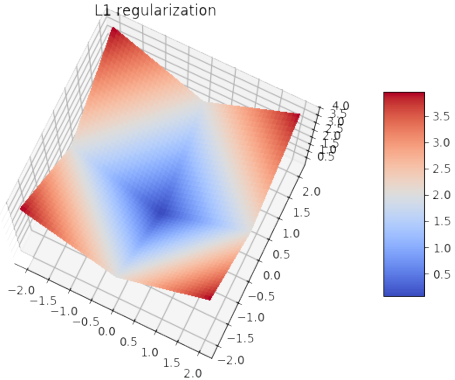

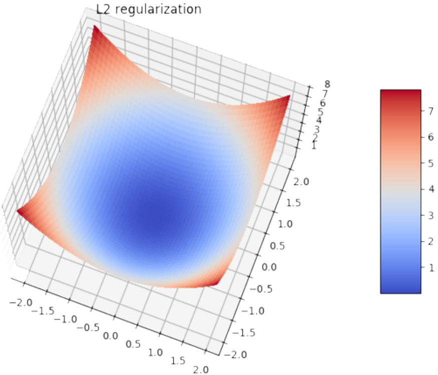

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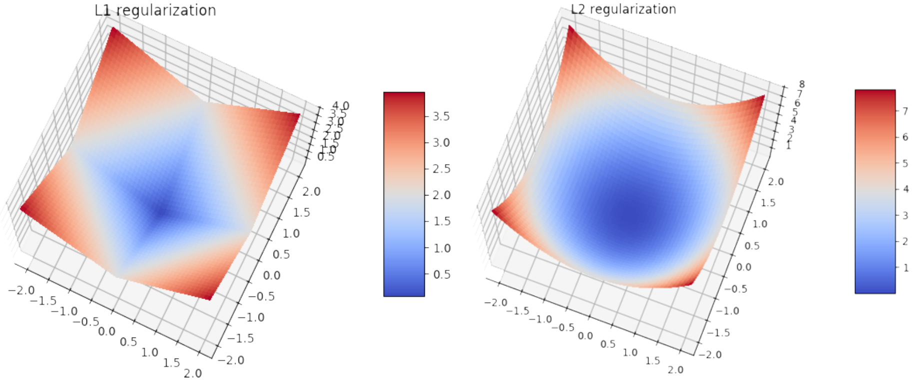

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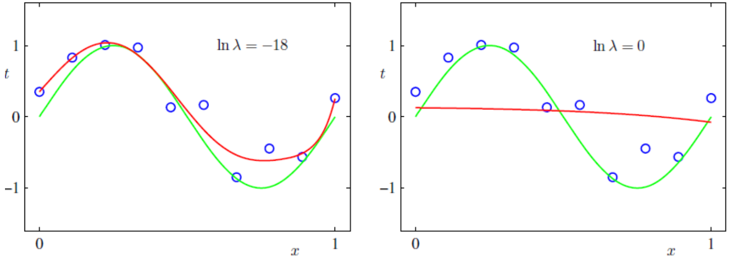
Effect of Regularization ($N = 10, M = 9$)



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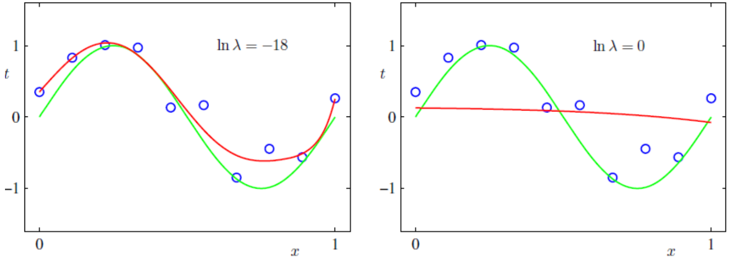

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$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
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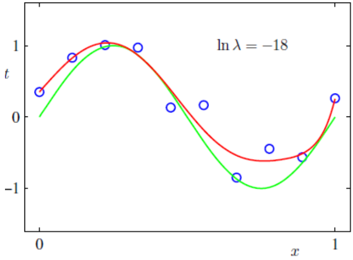

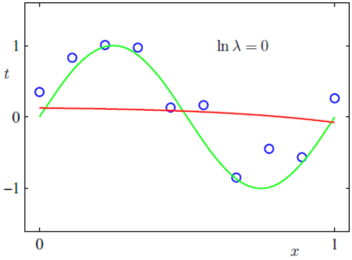

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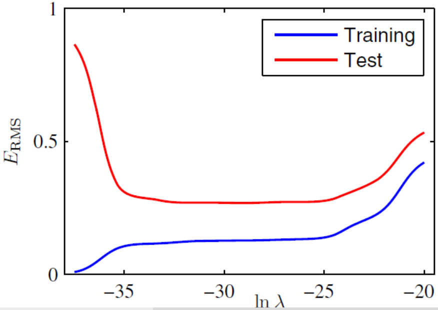

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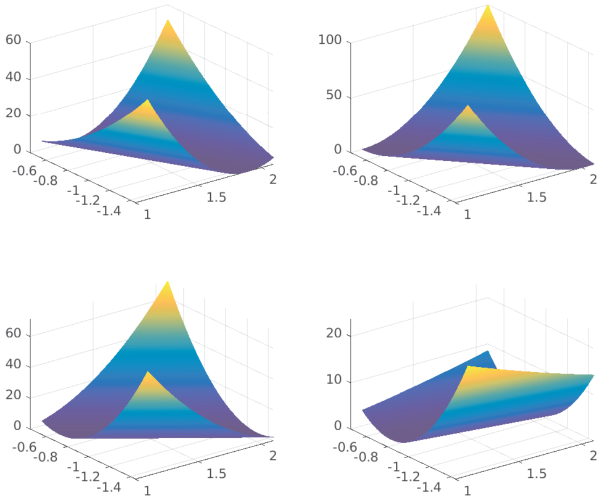
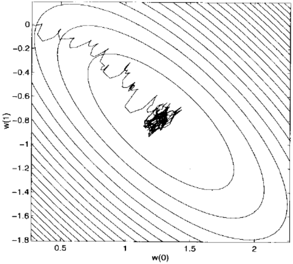
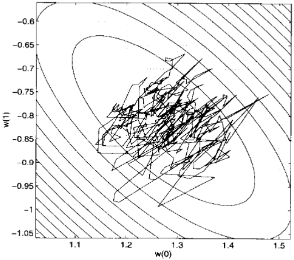
- $|\mathcal{B}| = N$: Steepest descent $|\mathcal{B}| = 1$: LMS Otherwise: SGD.

SGD Error Dynamics: $w_1 = 1.6, w_2 = -0.5$



Convergence of SGD





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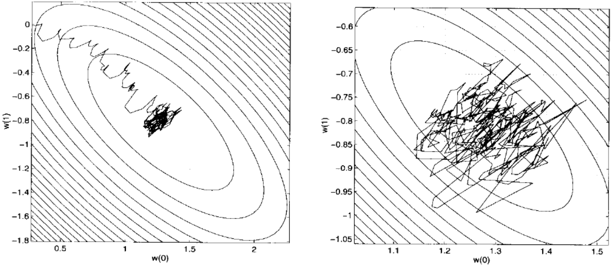
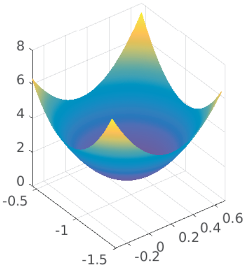


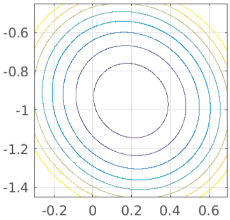
- SGD algorithm converges in mean:

$$\lim_{k\to\infty} \mathbb{E}[\mathbf{w}_k] \rightarrow (\mathbf{\Phi}^\mathsf{T}\mathbf{\Phi})^{-1}\mathbf{\Phi}^\mathsf{T}\mathbf{t} \qquad \eta \text{ is small enough}$$

- Expectation over multiple runs (k) converges to true solution for convex error surfaces, provided η is sufficiently small

Geometry of Error Surface vs Convergence Rate





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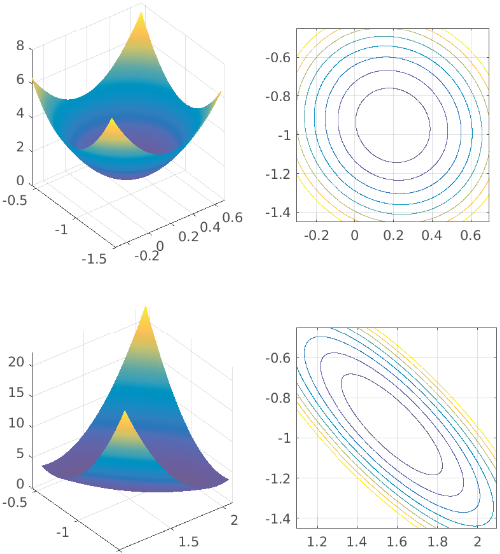

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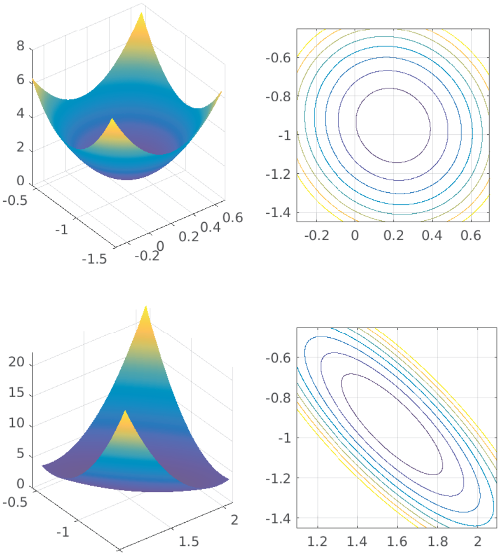

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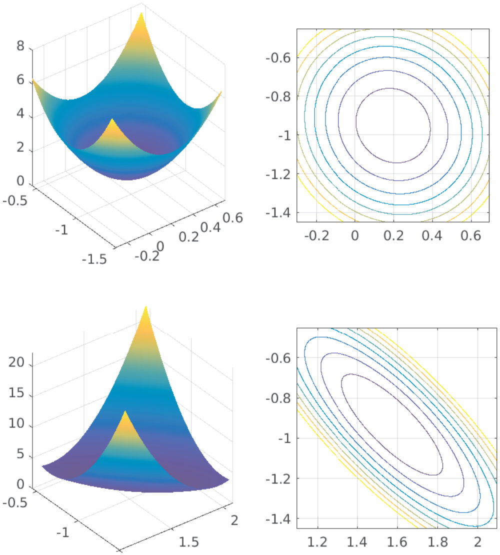

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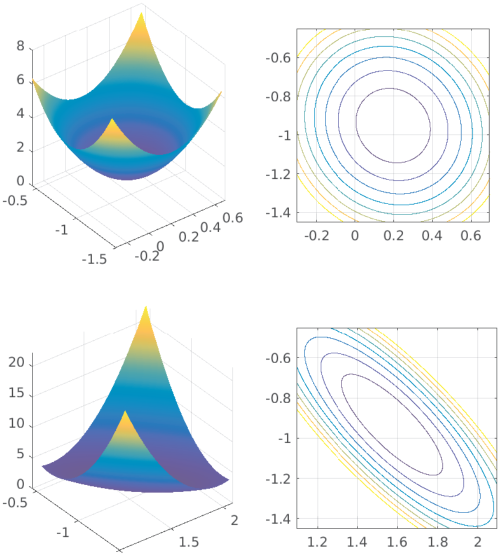

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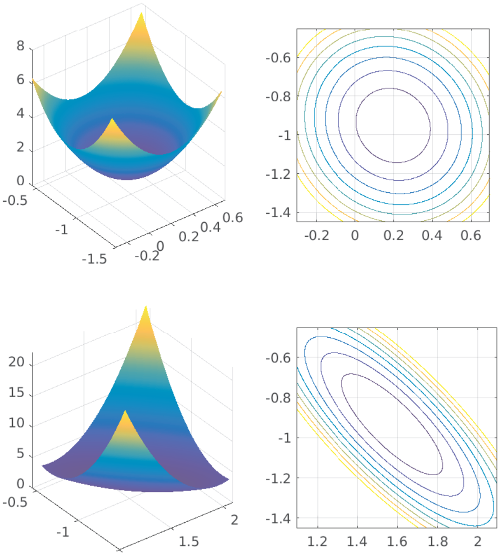

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- η has to be fixed based on steepest direction.
- Convergence along flatter dimension is too slow!

Newtons Method

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$$\mathbf{w}_{n+1} = \mathbf{w}_n + \Delta\mathbf{w}$$

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- Optimal update is given by $\Delta\mathbf{w} = -\frac{\nabla J(\mathbf{w}_n)}{\nabla^2 J(\mathbf{w}_n)}$

$$\mathbf{w}_{n+1} = \mathbf{w}_n - \mathbf{H}^{-1}(\mathbf{w}_n)\nabla J(\mathbf{w}_n) \qquad \mathbf{H}(\mathbf{w}_n) = \nabla^2 J(\mathbf{w}_n)$$

Homework - 1

- Apply Newtons method to steepest-descent algorithm to the optimal step size η, and check how many iterations are required for convergence.

$$\mathbf{w}^{new} = \mathbf{w}^{old} + \eta\, \mathbf{X}^{\mathsf{T}}(\mathbf{t} - \mathbf{X}\mathbf{w})\Big|_{\mathbf{w}=\mathbf{w}^{old}}$$

Homework - 2

- Suppose you are experimenting with L_1 and L_2 regularization. Further, imagine that you are running gradient descent and at some iteration your weight vector is $w = [1, \epsilon] \in \mathbb{R}^2$ where $\epsilon > 0$ is very small. With the help of this example explain why L_2 norm does not encourage sparsity i.e., it will not try to drive ϵ to 0 to produce a sparse weight vector. Give mathematical explanation.

Homework - 3

- Till now we have been considering a scalar target t from a vector of input observations $\mathbf{x}$. How do you extend this approach for regressing a vector of targets $\mathbf{t} = (t_1, t_2, \cdots t_P)$. Derive the closed form solutions and write sequential update equations using SGD.