Linear Models of Regression

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Regression

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$$\hat{t} = y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + w_2 x_2 + \cdots w_D x_D = \mathbf{w}^\mathsf{T}\mathbf{x}$$

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

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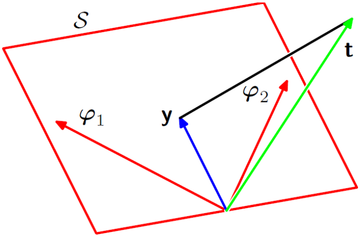
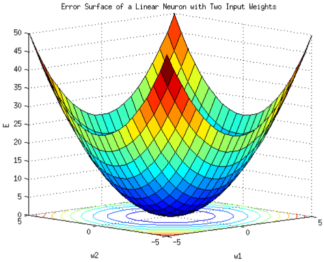
- Equating derivative w.r.t $\mathbf{w}$ to 0

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

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

Geometric Interpretation of Least Squares





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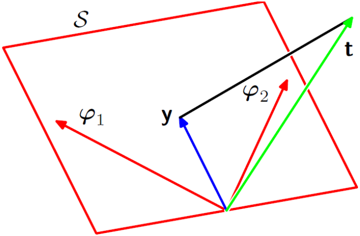

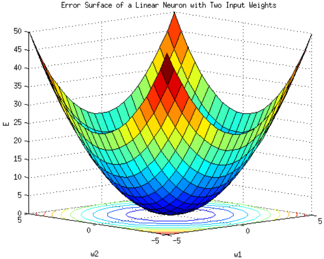

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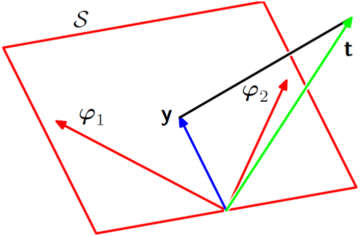

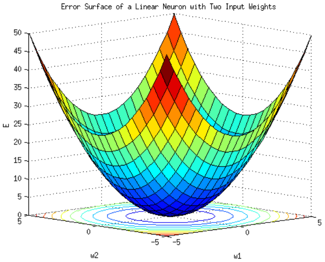

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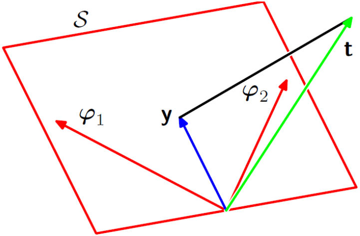

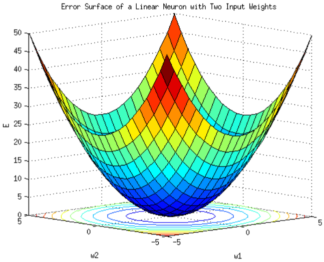

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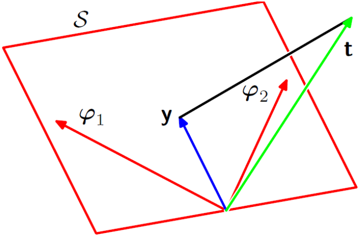

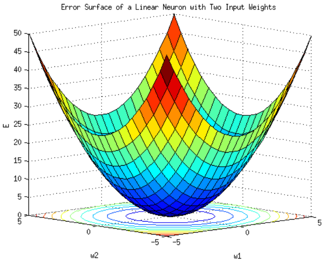

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- For the LS optimality criterion

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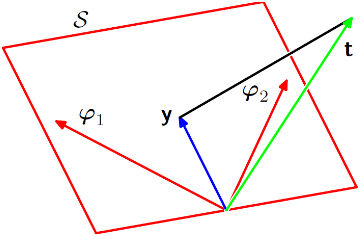

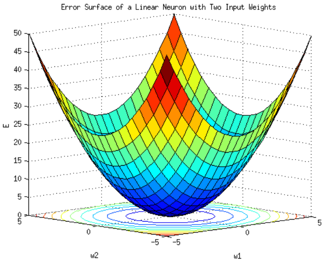

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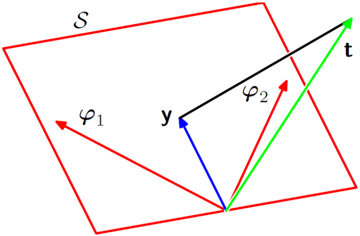

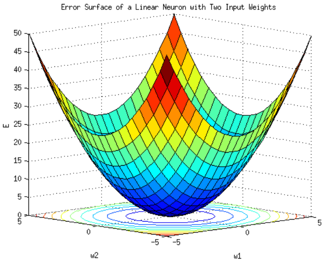

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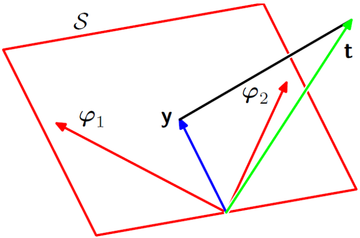

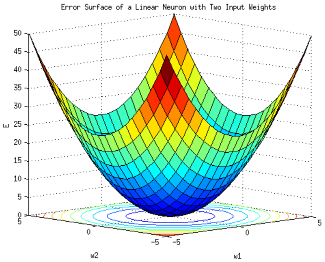

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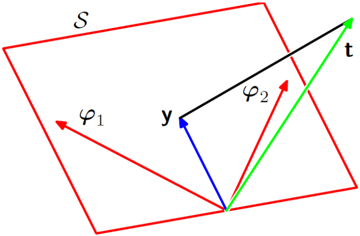

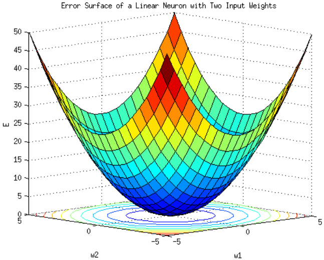

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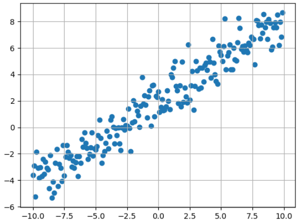
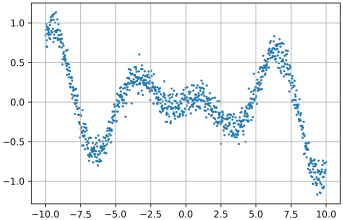
  - Also referred to as pseudo inverse sol.

Nonlinear Input-Output Relations



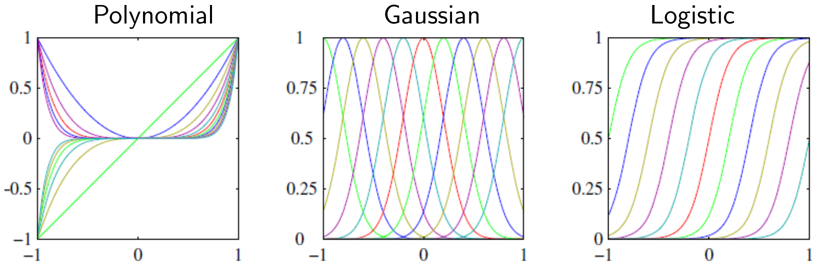


- Polynomial curve fitting can be used to model ninlinear i/o relation

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

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

Kernel Examples



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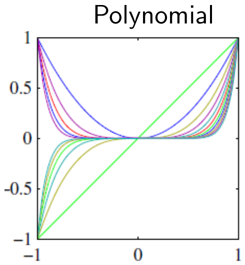
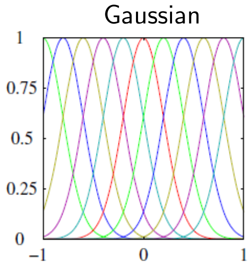
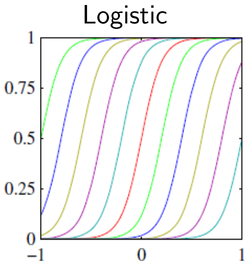


$$\phi_j(x) = x^j$$



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



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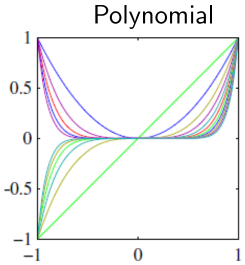

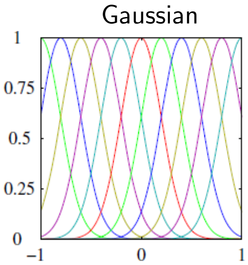

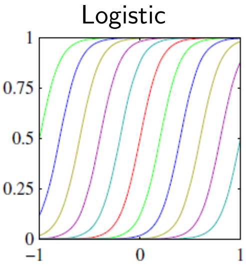

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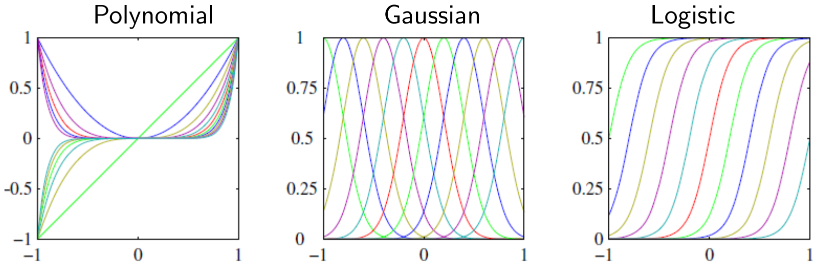

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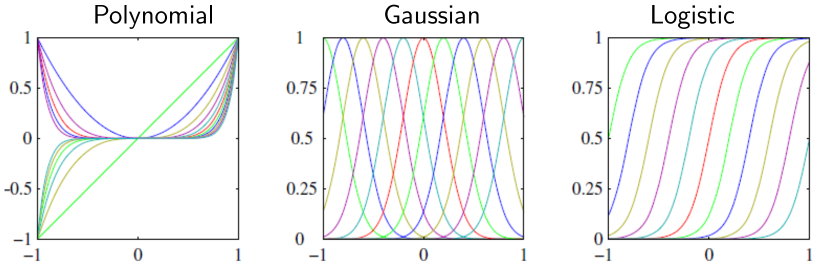

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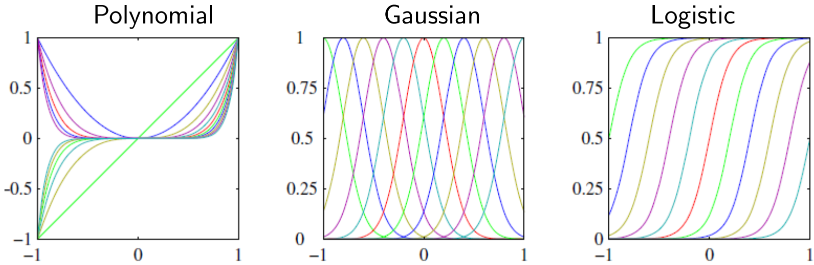

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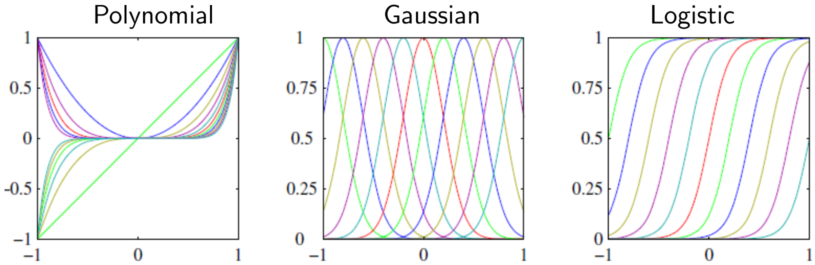

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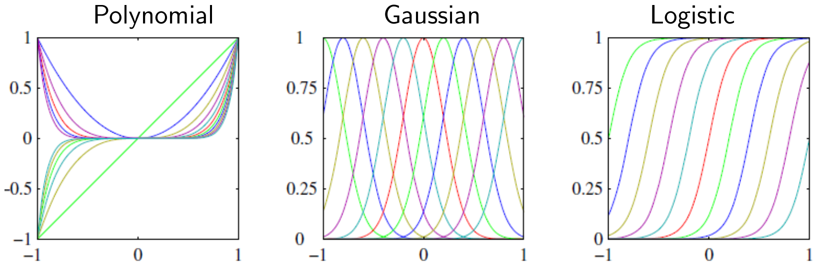

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  - Changes in one region of input space affect all other regions
  - Local kernels are preferable for functions with varying characteristics

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- $\mathbf{x}_n = [x_{n1} \ x_{n2}]^\mathsf{T} \in \mathbb{R}^2$ can be mapped using 2nd 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

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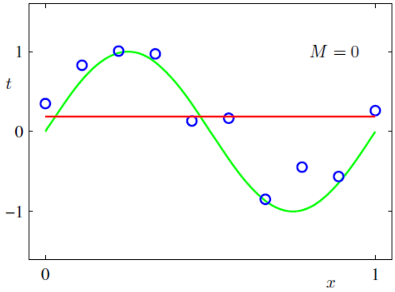
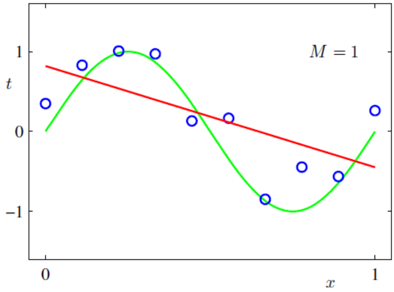
- The last layer of DNNs typically performs linear regression on $\phi(\mathbf{x}_n)$

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





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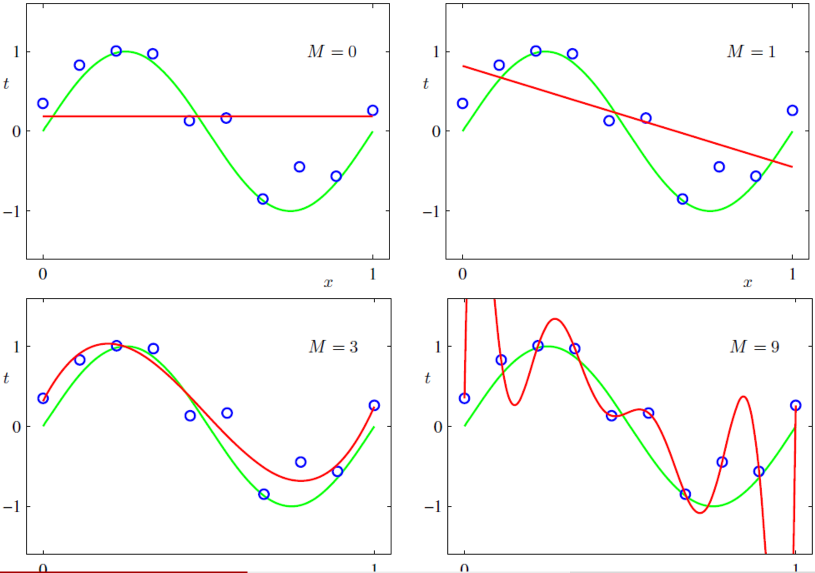

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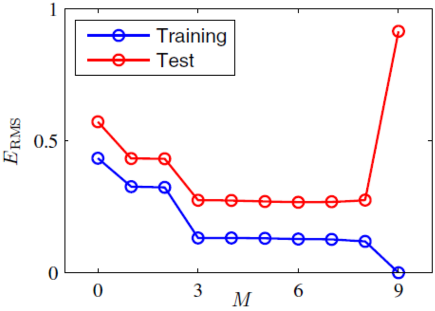

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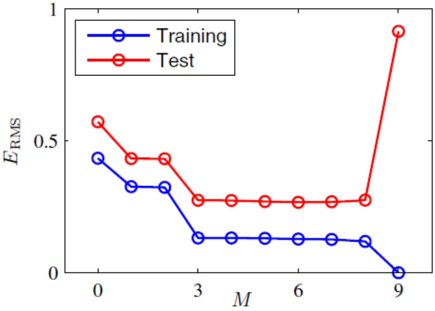

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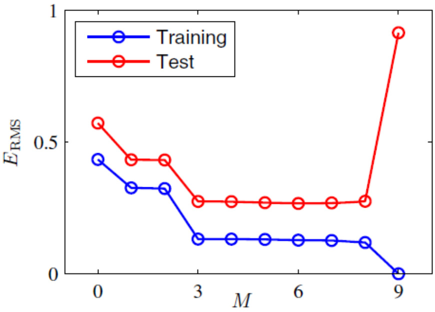

	$M=0$	$M=1$	$M=6$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
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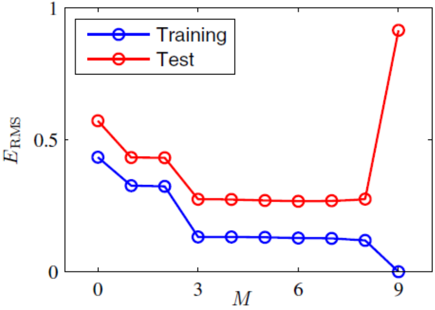

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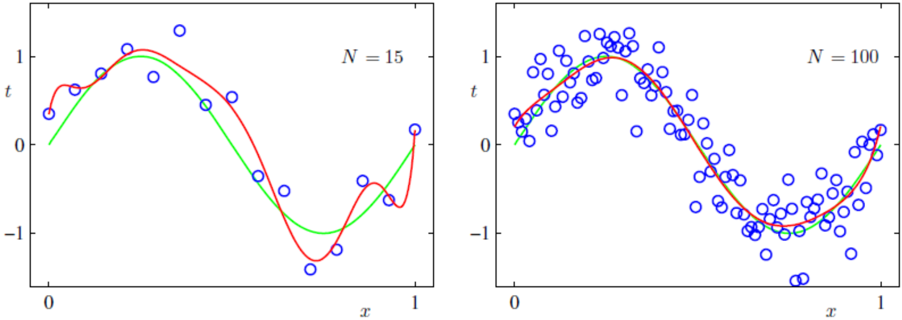
- Large amplitude weights with alternating polarity.
- $(\mathbf{\Phi}^T\mathbf{\Phi})$ may be ill conditioned

Amount of Training Data ($M = 9$)



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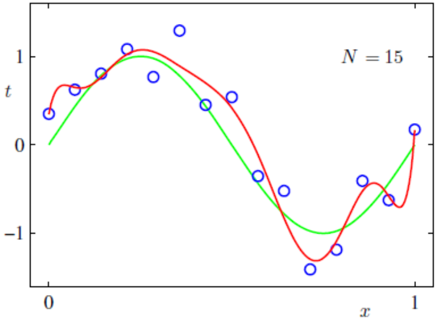

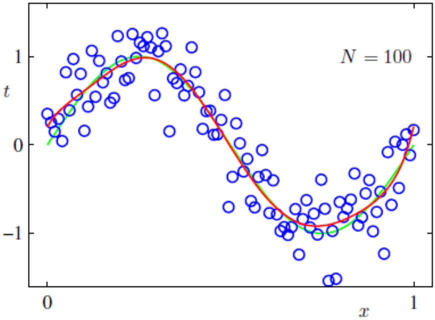

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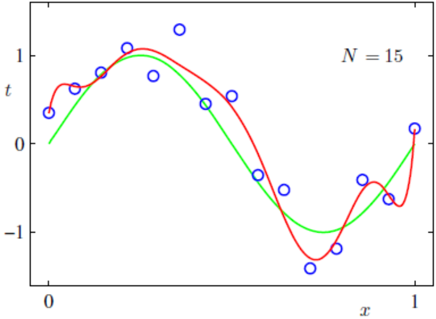

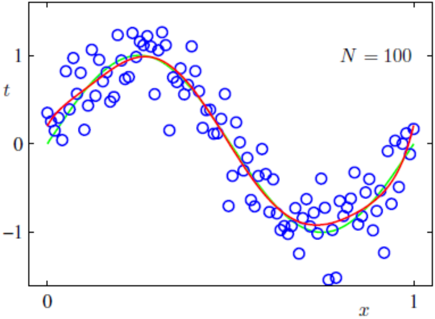

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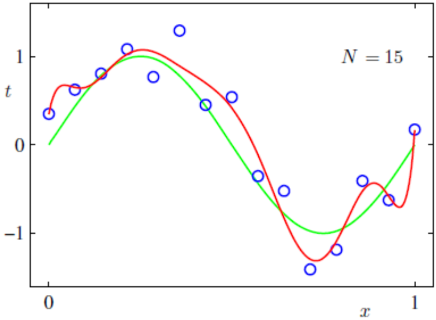

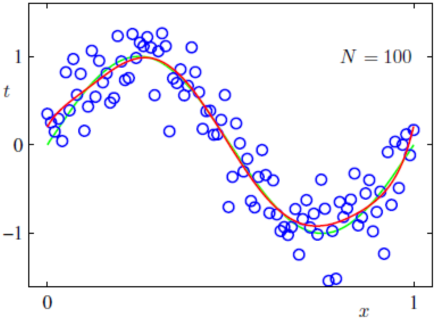

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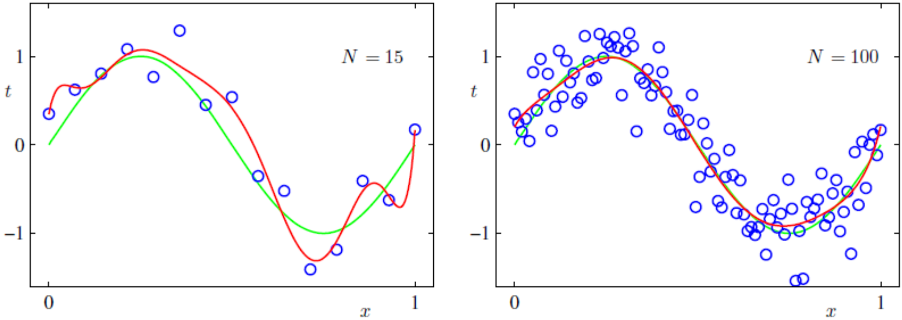

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- A way forward: arrest the growth of the model weights

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!

Modified Error Surface

$$J(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\Big(t_n - \mathbf{w}^{\mathsf{T}}\phi(\mathbf{x}_n)\Big)^2 + \lambda\|\mathbf{w}\|_p$$

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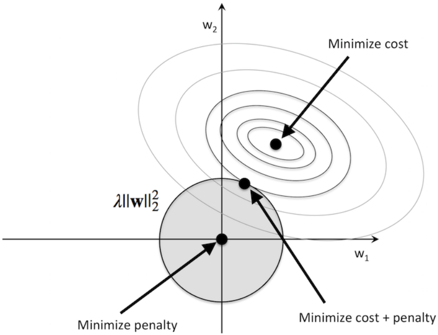

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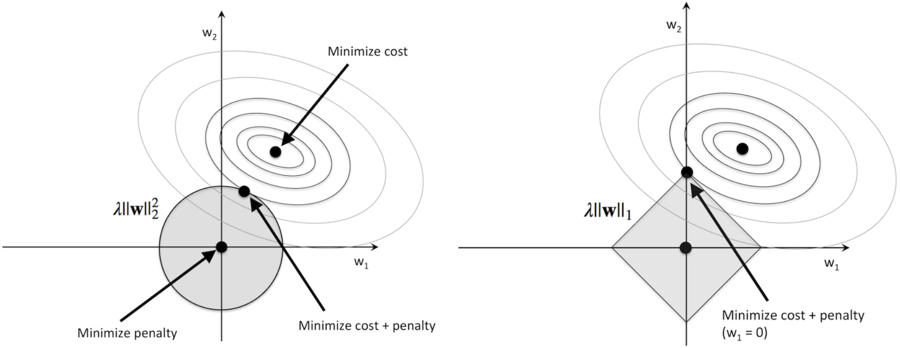
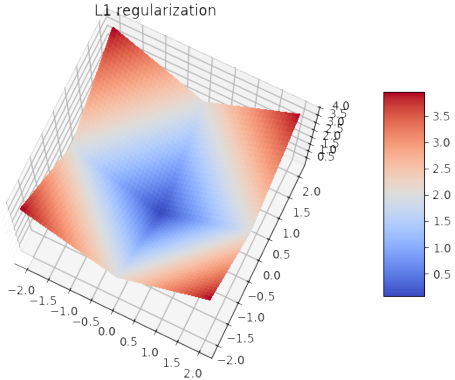


L_2 Regularizer　　L_1 Regularizer

L_1 vs L_2


L1 regularization
−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0
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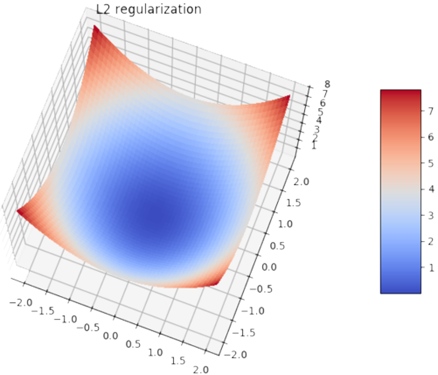
0.5 1.0 1.5 2.0 2.5 3.0 3.5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−2.0 −1.5 −1.0 −0.5 0.0 0.5 1.0 1.5 2.0
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1 2 3 4 5 6 7 8

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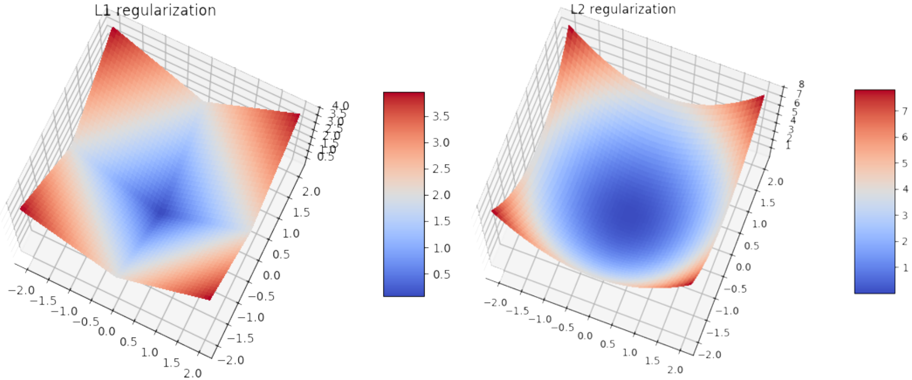

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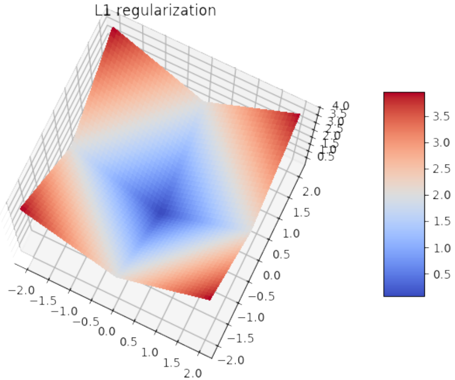

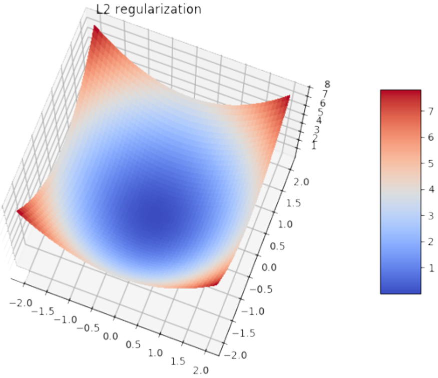

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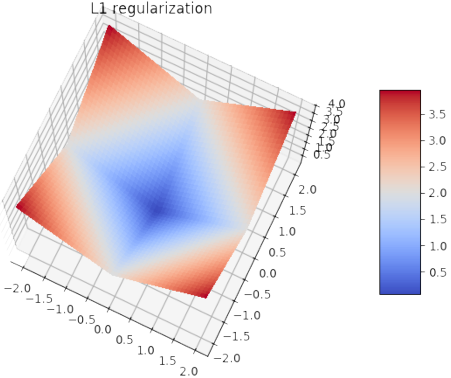

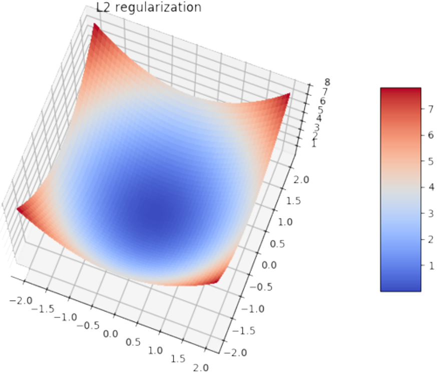

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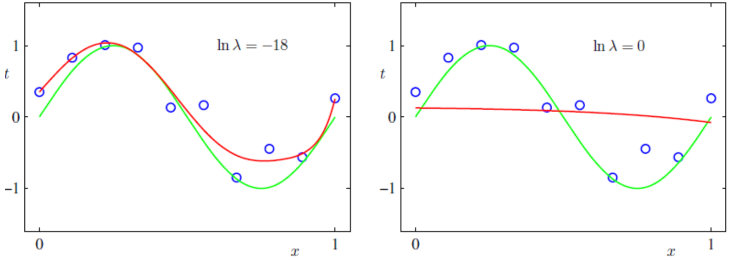
Effect of Regularization ($N = 10, M = 9$)



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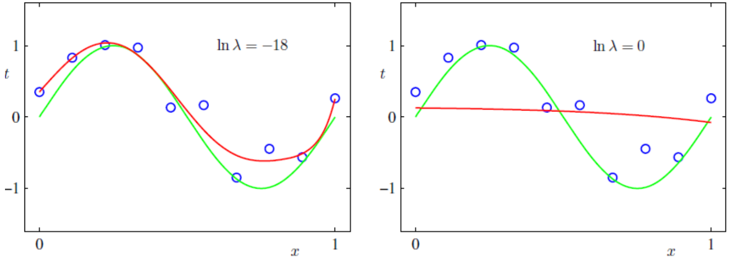

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
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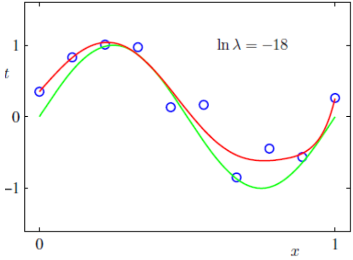

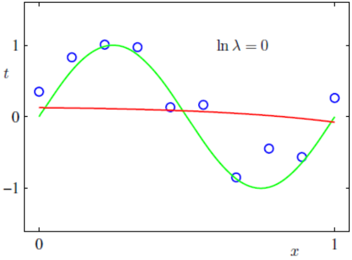

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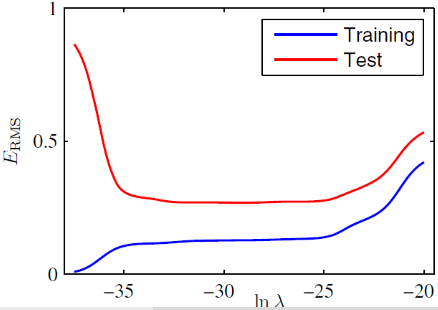

Sequential Learning

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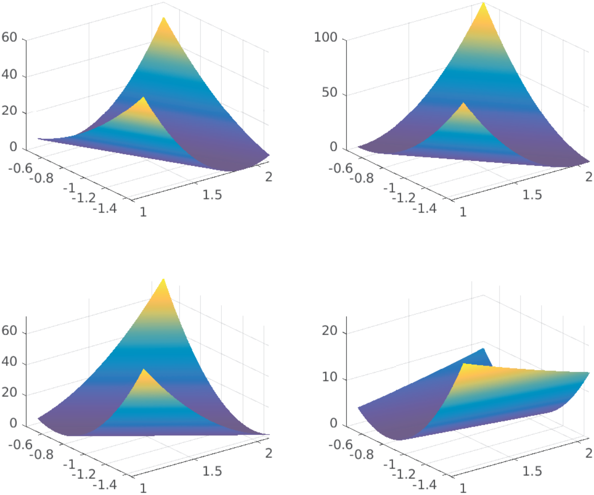
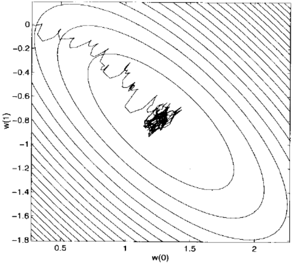
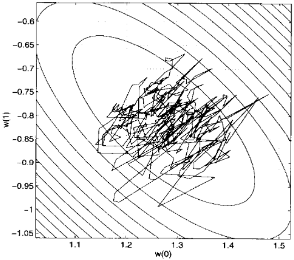
- $|\mathcal{B}| = N$: Steepest descent $\quad |\mathcal{B}| = 1$: LMS $\quad$ Otherwise: SGD.

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



Convergence of SGD





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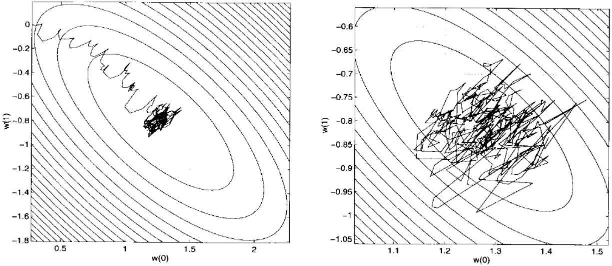
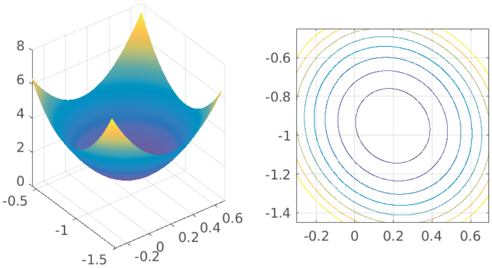


- SGD algorithm converges in mean:

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

- 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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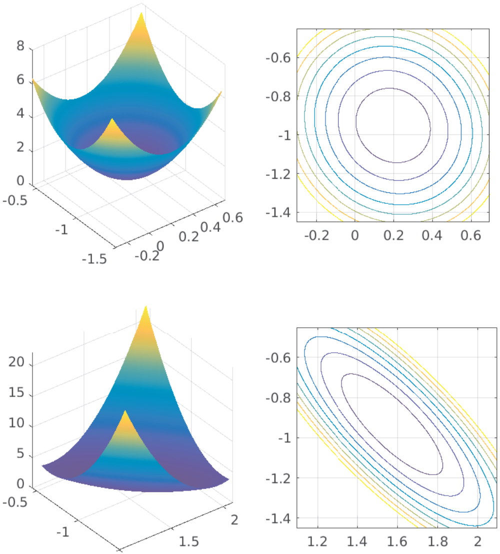

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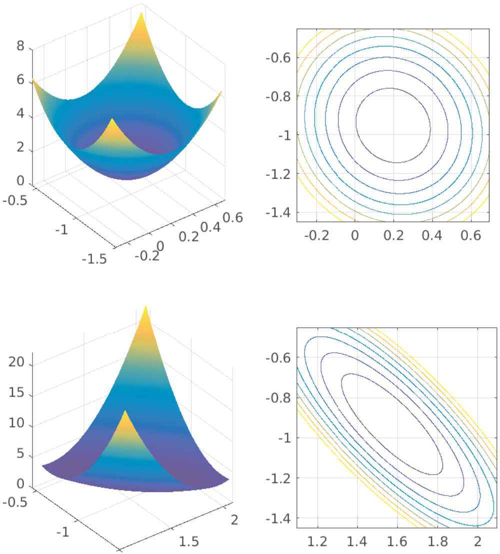

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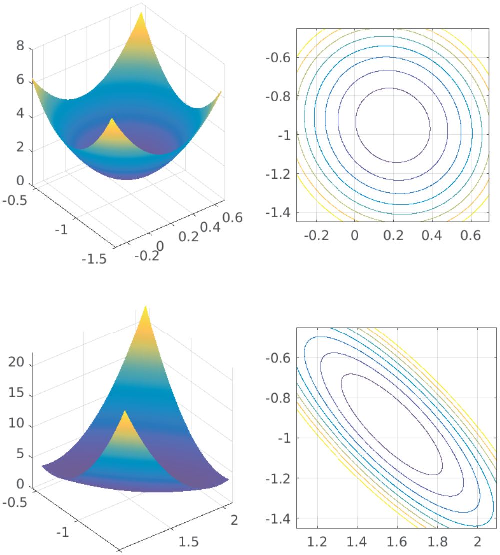

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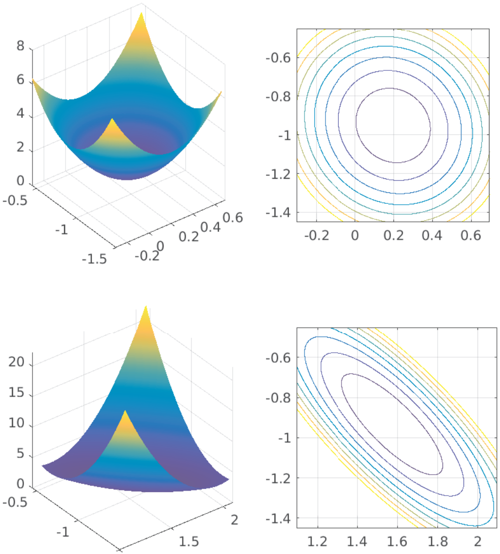

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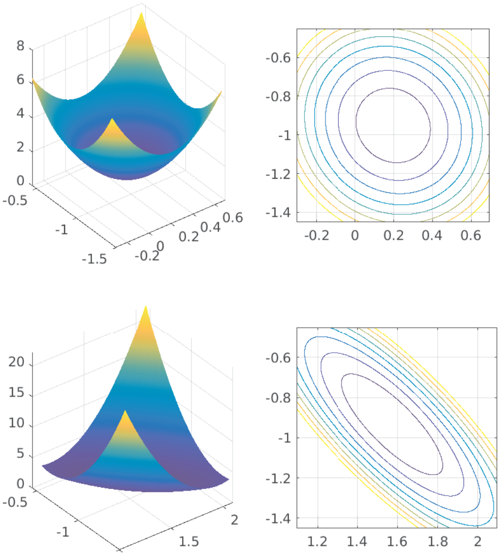

- Gradient magnitude depends on direction!
- η has to be fixed based on steepest direction.
- Convergence along flatter dimension is too slow!

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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.

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- $\mathbf{w}$ and β can be estimated to maximize likelihood $p(\mathbf{t}/\mathbf{X}, \mathbf{w}, \beta)$

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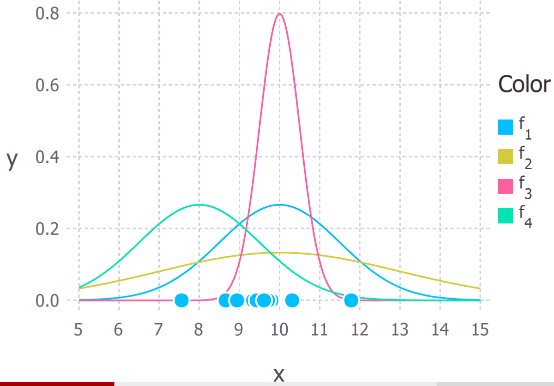

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- Estimate w to maximize $\log p(\mathbf{w}/\mathbf{t})$

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- $\mathbf{m}_N$ and $\mathbf{\Sigma}_N$ can be evaluated by completing quadratic term of exp()

$$\mathbf{m}_N = \mathbf{\Sigma}_N \left(\mathbf{\Sigma}_0^{-1}\mathbf{m}_0 + \beta\mathbf{\Phi}^\mathsf{T}\mathbf{t} \right)$$

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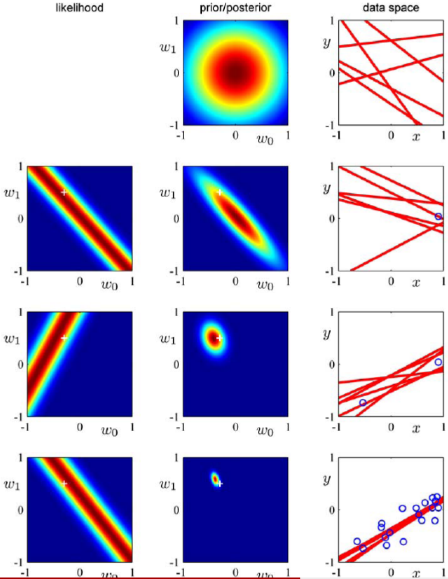
- The posterior stats can be updated after observing $(\mathbf{x}_{n+1}, t_{n+1})$ as

$$\mathbf{m}_{n+1} = \boldsymbol{\Sigma}_{n+1}\left(\boldsymbol{\Sigma}_n^{-1}\mathbf{m}_n + \beta\phi(\mathbf{x}_{n+1})t_{n+1}\right)$$
$$\boldsymbol{\Sigma}_{n+1}^{-1} = \boldsymbol{\Sigma}_n^{-1} + \beta\phi(\mathbf{x}_{n+1})\phi^{\mathsf{T}}(\mathbf{x}_{n+1})$$

Bayes Updates Illustration: $t = a_0 + a_1 x + \epsilon$



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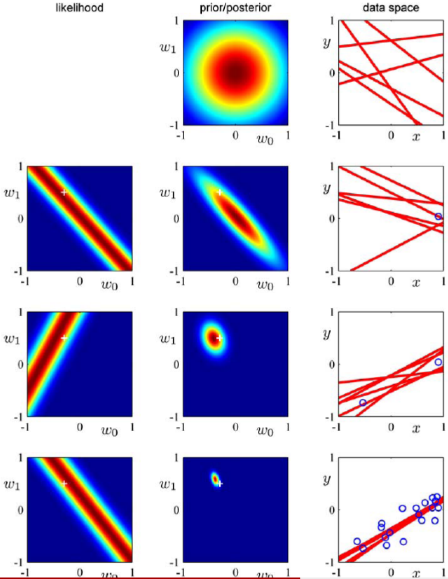

- Actual targets are generated as

$$t = 0.5x - 0.3 + \epsilon$$

$$x \in \mathcal{U}[-1\ 1] \qquad \epsilon \in \mathcal{N}(0, 0.2^2)$$

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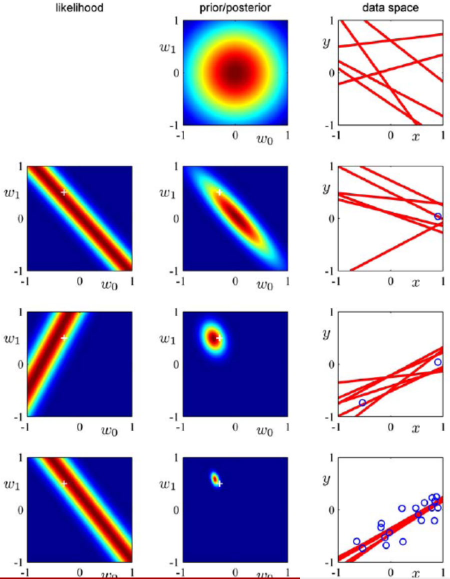

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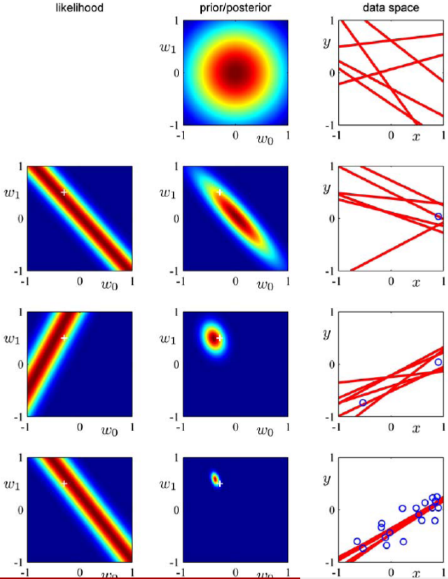

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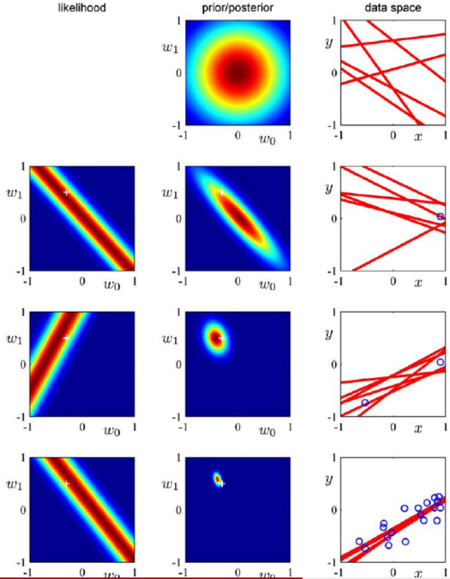

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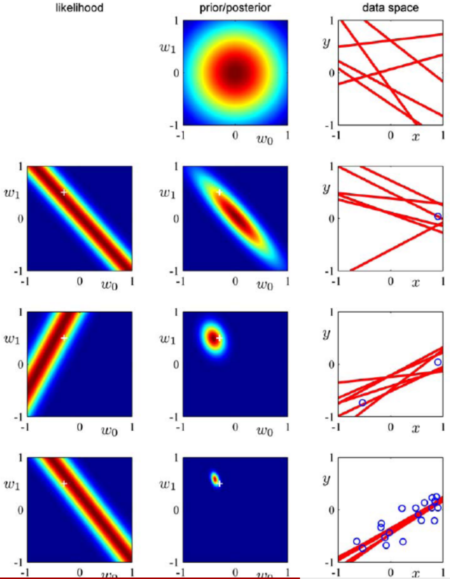

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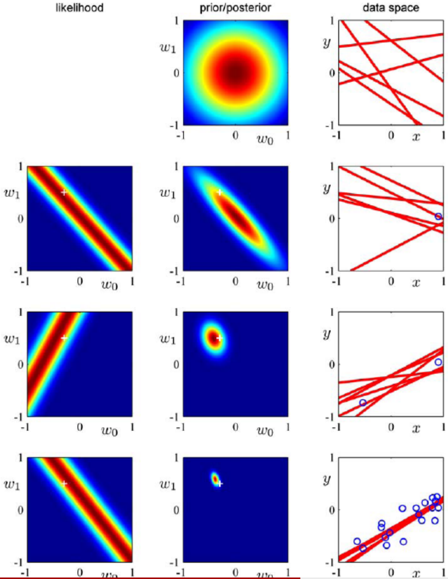

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- Lines converge as data increase

Homework

- Derive the statistics of the posterior distribution $p(\mathbf{w}/\mathbf{t})$ by completing the quadratic term of exp(.)
- Given a Gaussian marginal distribution for $\mathbf{x}$ and a Gaussian conditional distribution for y in the form

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}/\mu, \mathbf{\Lambda})$$
$$p(\mathbf{y}/\mathbf{x}) = \mathcal{N}(\mathbf{y}/\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1})$$

show that the marginal distribution of $\mathbf{y}$ and conditional distribution of $\mathbf{x}$ are given by

$$p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}/\mathbf{A}\mu + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1}\mathbf{A}^{\mathsf{T}}\right)$$
$$p(\mathbf{x}/\mathbf{y}) = \mathcal{N}\left(\mathbf{x}/\mathbf{\Sigma}\left(\mathbf{A}^{\mathsf{T}}\mathbf{L}(\mathbf{y}-\mathbf{b}) + \mathbf{\Lambda}\mu\right), \mathbf{\Sigma}\right)$$

where $\mathbf{\Sigma} = \left(\mathbf{\Lambda} + \mathbf{A}^{\mathsf{T}}\mathbf{L}\mathbf{A}\right)^{-1}$

Predictive Distributions

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- Given a training set of N points $(\mathbf{x}_{1:N}, t_{1:N})$, predict target distribution for a new input $\mathbf{x}_0$

$$\begin{aligned} p(t_0/\mathbf{x}_0, \mathbf{X}, \mathbf{t}, \alpha, \beta) &= \int p(t_0, \mathbf{w}/\mathbf{x}_0, \mathbf{X}, \mathbf{t}, \alpha, \beta) d\mathbf{w} \\ &= \int p(t_0/\mathbf{w}, \mathbf{x}_0, \beta) p(\mathbf{w}/\mathbf{X}, \mathbf{t}, \alpha, \beta) d\mathbf{w} \end{aligned}$$

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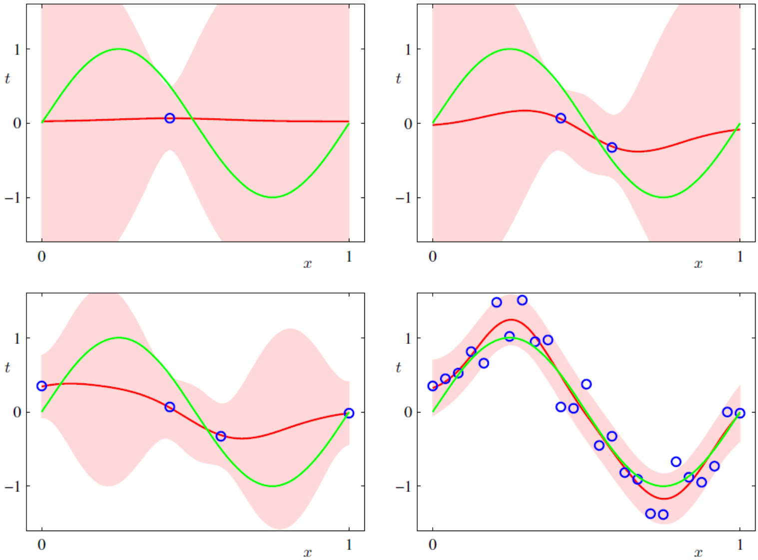
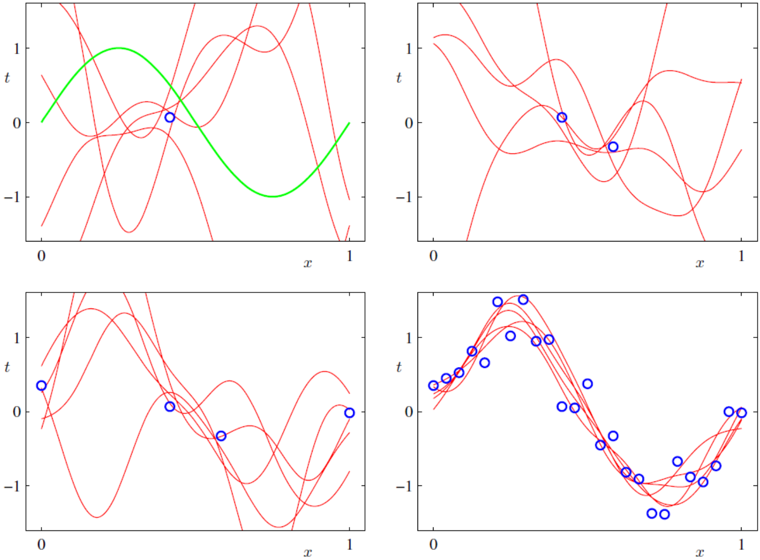
Predictive Distribution: $t = \sin(2\pi x) + \epsilon$



Curves $y(x, \mathbf{w})$ Sampled from Posterior $p(\mathbf{w}/\mathbf{t})$



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  - Parameters $\mathbf{w}$ depend on training set - point estimate not enough
  - MAP estimation assigns a distribution to $\mathbf{w}$: $p(\mathbf{w}/\mathbf{t}, \mathbf{X}, \alpha, \beta)$
  - Predict target distribution for a test-point x_0: $p(t_0/x_0, \mathbf{t}, \mathbf{X}, \alpha, \beta)$

Summary of Linear Models of Regression

- Linear in model parameters **w**.
  - If **x** and t are linearly related $\hat{t} = \mathbf{w}^\mathsf{T}\mathbf{x}$
  - If relationship is not linear: $\hat{t} = \mathbf{w}^\mathsf{T}\phi(\mathbf{x})$
  - LS criterion leads to pseudo-inverse solution: $\mathbf{w}_* = (\mathbf{\Phi}^\mathsf{T}\mathbf{\Phi})^{-1}\mathbf{\Phi}^\mathsf{T}\mathbf{t}$
  - Regularize **w** to avoid over-fitting: $\mathbf{w}_* = (\mathbf{\Phi}^\mathsf{T}\mathbf{\Phi} + \lambda\mathbf{I})^{-1}\mathbf{\Phi}^\mathsf{T}\mathbf{t}$
  - Gradient descent algorithms can be used for sequential learning
- Probabilistic interpretation to regression
  - Point estimate of target does not hold for one-to-many maps
  - ML estimation assigns a distribution to the target $p(t_n/y(\mathbf{w}, \mathbf{x}_n), \beta^{-1})$
  - Parameters **w** depend on training set - point estimate not enough
  - MAP estimation assigns a distribution to **w**: $p(\mathbf{w}/\mathbf{t}, \mathbf{X}, \alpha, \beta)$
  - Predict target distribution for a test-point x_0: $p(t_0/x_0, \mathbf{t}, \mathbf{X}, \alpha, \beta)$
  - Predictive uncertainty depends on x_0 and is smallest in the neighborhood of train data points.

Homework

- For Gaussian likelihood and Gaussian posterior, prove that the he predictive distribution is Gaussian and is given by

$$p(t_0/\mathbf{x}_0, \mathbf{X}, \mathbf{t}, \alpha, \beta) = \mathcal{N}\left(t_0/\mathbf{m}_N^T \phi(\mathbf{x}_0), \sigma_N^2(\mathbf{x}_0)\right)$$
$$\sigma_N^2(\mathbf{x}_0) = \frac{1}{\beta} + \boldsymbol{\phi}^{\mathsf{T}}(\mathbf{x}_0)\boldsymbol{\Sigma}_N \phi(\mathbf{x}_0)$$

- Prove that the predictive uncertainty deceases with increase in training data, i.e., predictive distribution gets narrower with additional training points

$$\sigma_{N+1}^2(\mathbf{x}_0) \leq \sigma_N^2(\mathbf{x}_0)$$

Thank You!