Linear Regression

Machine Learning

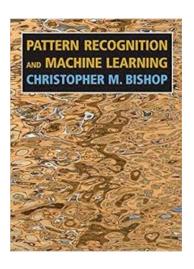
Daniele Loiacono



References

☐ This slides are based on material of prof. Marcello Restelli

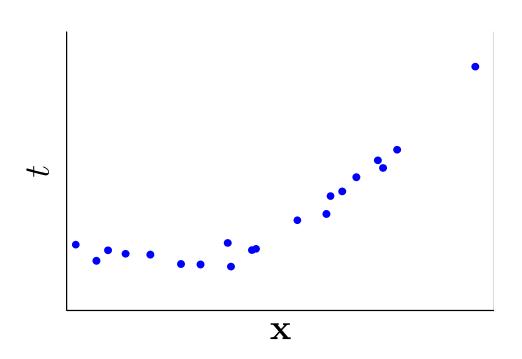
- ☐ Pattern Recognition and Machine Learning, Bishop
 - ► Chapter 1 (1.1, 1.2, 1.3)
 - ► Chapter 3 (3.1, 3.3)



What is regression?

Learn an **approximation** of function f(x) that maps input x to a continuous output t from a dataset \mathcal{D}

$$\mathcal{D} = \{\langle x, t \rangle\} \Rightarrow t = f(x)$$

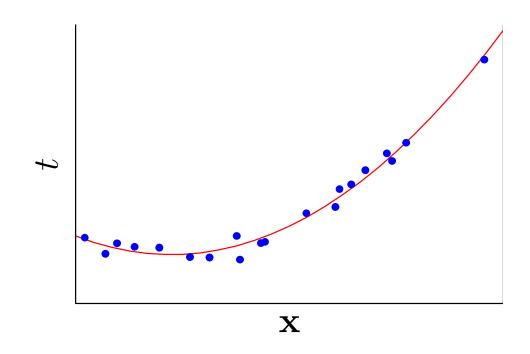


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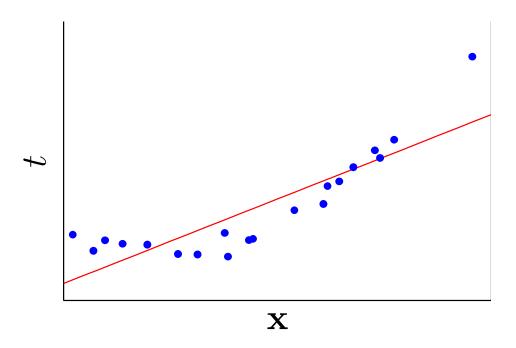
$$\mathcal{D} = \{\langle x, t \rangle\} \Rightarrow t = f(x)$$

- ▶ How do we model *f*?
- ► How do we evaluate our approximation?
- ► How do we optimize our approximation?



Linear Regression

- \square In linear regression, f(x) is modeled with linear functions
 - Linear models can be easily explained
 - ▶ A linear regression problem can be solved analytically
 - Linear functions can be extended to model also non-linear relationships
 - More sophisticated methods are based on linear regression

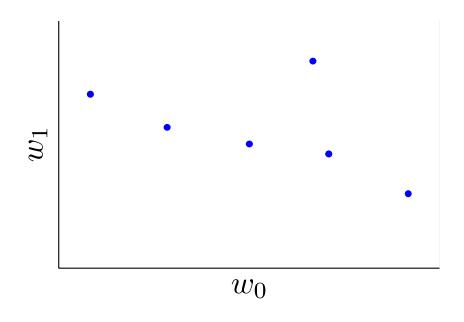


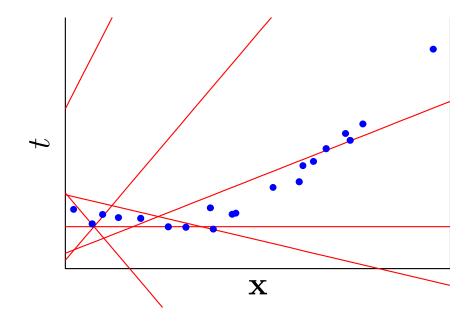
Linear Regression: model

☐ The simplest linear model can be defined as:

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{D-1} w_j x_j = \mathbf{w}^T \mathbf{x}$$

- $\mathbf{x} = (1, x_1, \dots, x_{D-1})$
- $ightharpoonup w_0$ is called bias parameter





Linear Regression: loss function and optimization

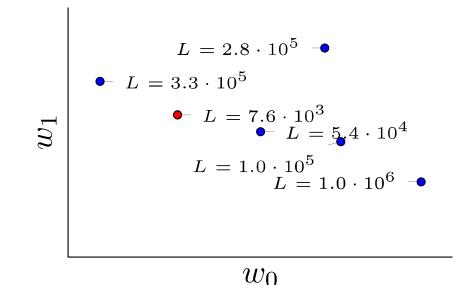
□ A convenient error loss function is the sum of squared errors (SSE):

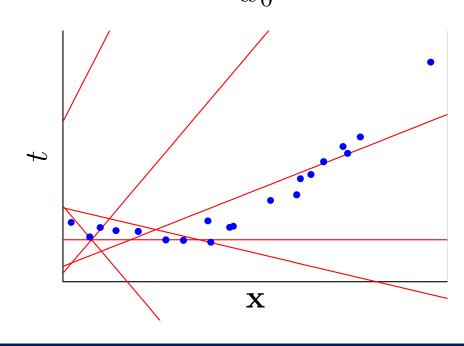
$$L(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} (y(x_n, \mathbf{w}) - t_n)^2$$

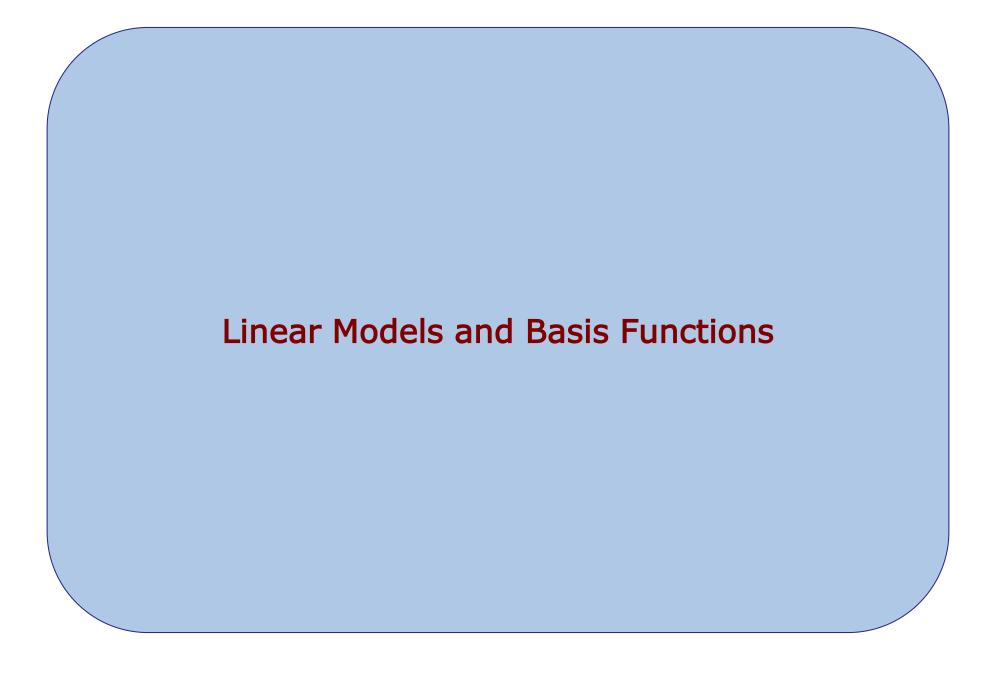
▶ the sum in £ is also called residual sum of squares (RSS) and can be written as the sum of residual errors:

$$RSS(\mathbf{w}) = \|\boldsymbol{\epsilon}\|_{2}^{2} = \sum_{i=1}^{N} \epsilon_{i}^{2}$$

► closed-form optimization of £ can be easily obtained





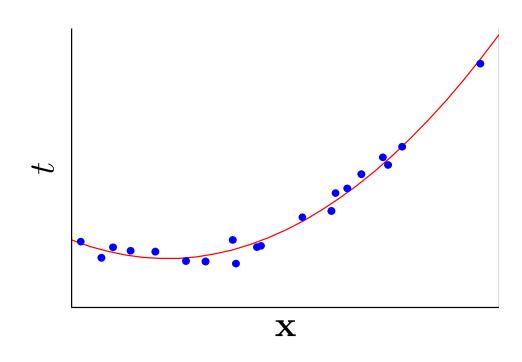


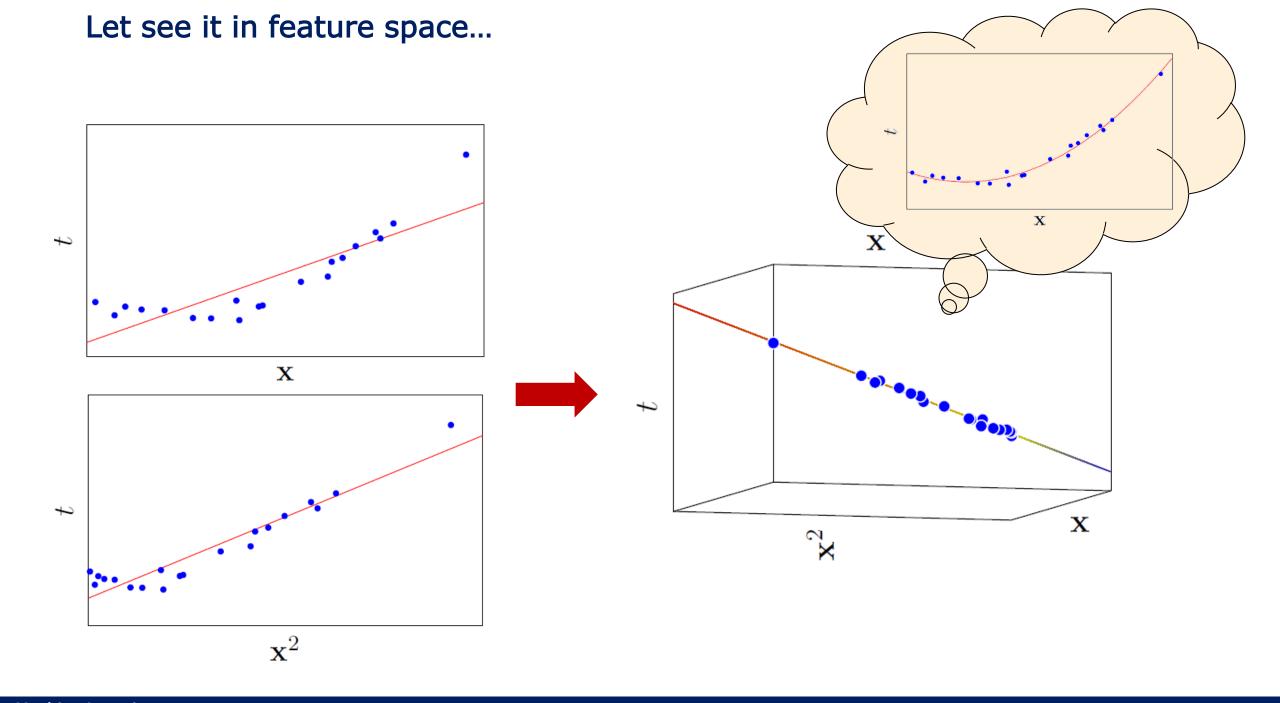
Linear Models

- ☐ A linear combination of the input variables is not enough to model data...
- ... but we just need a regression model that is linear in the parameters
- We can define a model using non-linear basis functions:

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

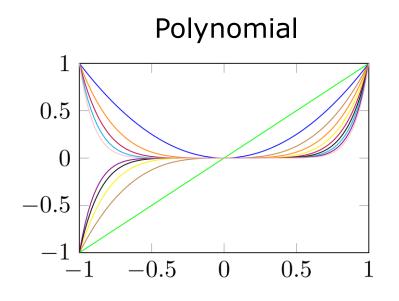
$$\phi(\mathbf{x}) = (1, \phi_1(\mathbf{x}), \dots, \phi_{M-1}(\mathbf{x}))^T$$



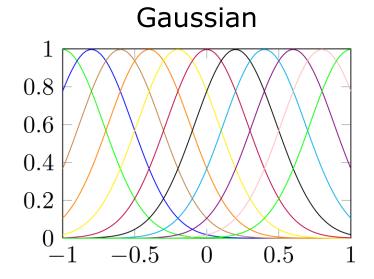


Basis Functions

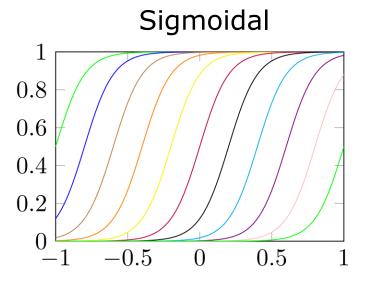
■ Some examples of basis function (assuming single-variable input)



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



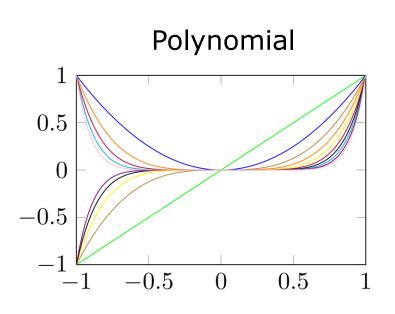
$$\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2\sigma^2}\right)$$
 $\phi_j(x) = \frac{1}{1+\exp\left(\frac{\mu_j-x}{\sigma}\right)}$



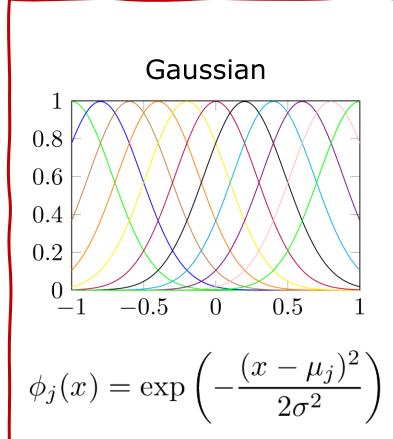
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Basis Functions

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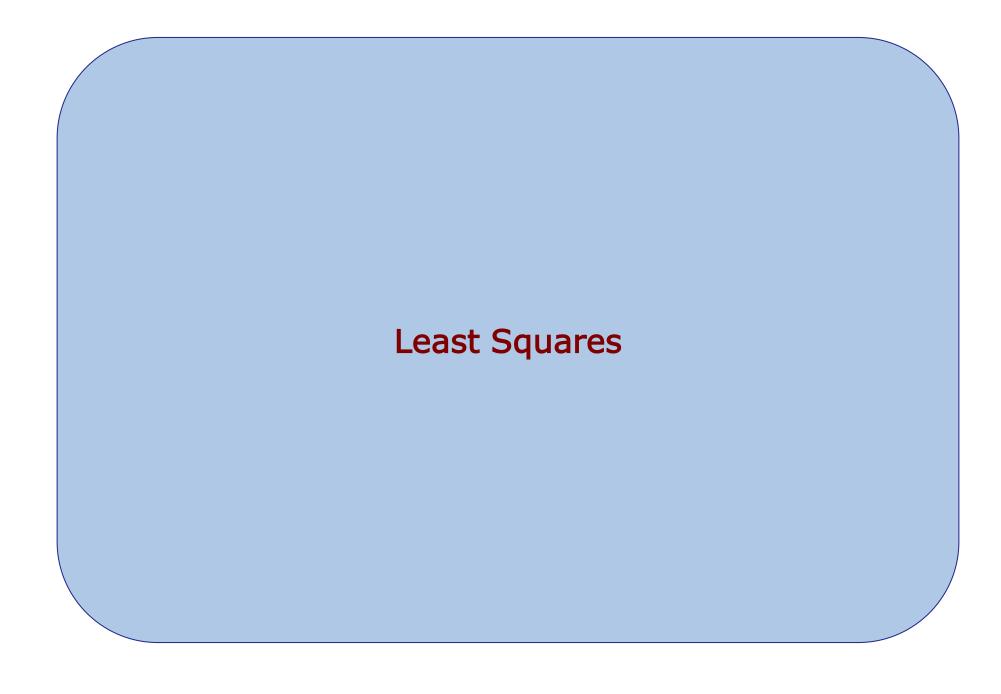
$0.4 \begin{vmatrix} 0.2 \\ 0.2 \end{vmatrix}$ $-1 \quad -0.5 \quad 0 \quad 0.5 \quad 1$ $\phi_j(x) = \frac{1}{1 + \exp\left(\frac{\mu_j - x}{\sigma}\right)}$

Sigmoidal

0.8

0.6

LOCAL



Ordinary Least Squares

□ For linear models, a closed-form optimization of the RSS, known as **least squares**, starting from the matrix form of the loss function:

$$L(\mathbf{w}) = \frac{1}{2}RSS(\mathbf{w}) = \frac{1}{2}(\mathbf{t} - \mathbf{\Phi}\mathbf{w})^{T}(\mathbf{t} - \mathbf{\Phi}\mathbf{w})$$

• where $\Phi = (\phi(\mathbf{x}_1), \dots, \phi(\mathbf{x}_N))^T$ and $\mathbf{t} = (t_1, \dots, t_N)^T$

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- \square We can compute first a second derivative of $\mathcal{L}(w)$ to find the optimal w

$$\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = -\mathbf{\Phi}^T \left(\mathbf{t} - \mathbf{\Phi} \mathbf{w} \right) \qquad \qquad \frac{\partial^2 L(\mathbf{w})}{\partial \mathbf{w} \partial \mathbf{w}^T} = \mathbf{\Phi}^T \mathbf{\Phi}$$

$$\hat{\mathbf{w}}_{OLS} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{t}$$

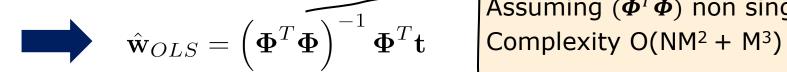
Ordinary Least Squares

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Assuming $(\boldsymbol{\Phi}^T\boldsymbol{\Phi})$ non singular

Sequential Learning

- ☐ Closed-form optimization (OLS) is not feasible with large dataset
- ☐ Instead, a **stochasitcs** (or s**equential**) gradient descent is possible
- ☐ Least Mean Square (LMS) algorithm:

$$L(\mathbf{x}) = \sum_{n} L(x_n)$$

$$\mathbf{w}^{(n+1)} = \mathbf{w}^{(n)} - \alpha^{(n)} \nabla L(x_n)$$

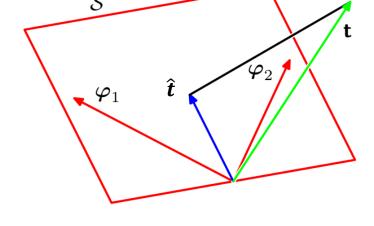
$$\Rightarrow \mathbf{w}^{(n+1)} = \mathbf{w}^{(n)} - \alpha^{(n)} \left(\mathbf{w}^{(n)}^T \boldsymbol{\phi}(\mathbf{x}_n) - t_n \right) \boldsymbol{\phi}(\mathbf{x}_n)$$

 $\triangleright \alpha$ is called learning rate and to guarantee convergence:

$$\sum_{n=0}^{\infty} \alpha^{(n)} = +\infty \qquad \qquad \sum_{n=0}^{\infty} \alpha^{(n)^2} < +\infty$$

Geometric Interpreation of OLS

- ☐ Let *t* be the N-dimensional target vector
- \Box Let φ_i be the *j*-th column of matrix Φ
 - $ightharpoonup \varphi_1, ..., \varphi_M$ identify a linear subspace \mathcal{S}
- \Box Let \hat{t} be the N-dimensional vector computed as Φw
 - $ightharpoonup \hat{t}$ is a linear combination of φ_i and lies in \mathcal{S}
- lacksquare OLS finds \hat{t} minimizing the SSE with respect to t
 - $ightharpoonup \hat{t}$ represents the projection of t onto the subspace S



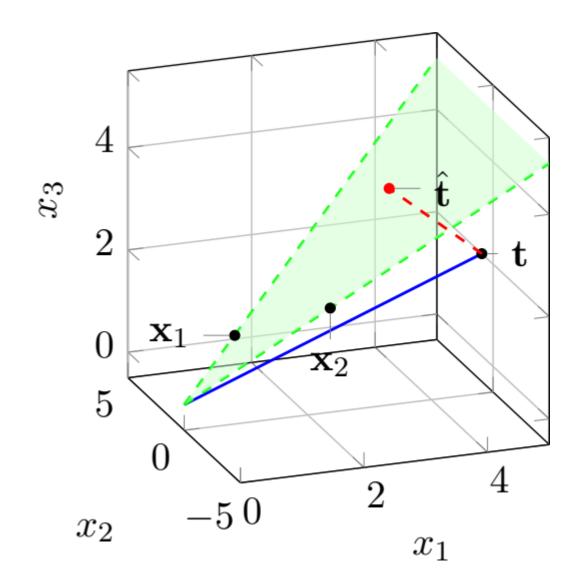
$$\hat{\mathbf{t}} = \mathbf{\Phi} \hat{\mathbf{w}} = \mathbf{\Phi} \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{t}$$
Hat Matrix (H)

Geometric Interpreation of OLS: an example

 \square Let N=3 and M=2

$$\mathbf{\Phi} = \mathbf{X} = \begin{pmatrix} 1 & 2 \\ 1 & -2 \\ 1 & 2 \end{pmatrix}$$

$$\mathbf{t} = \begin{pmatrix} 5 \\ 1 \\ 2 \end{pmatrix} \qquad \hat{\mathbf{t}} = \begin{pmatrix} 3.5 \\ 1 \\ 3.5 \end{pmatrix}$$



Multiple Outputs

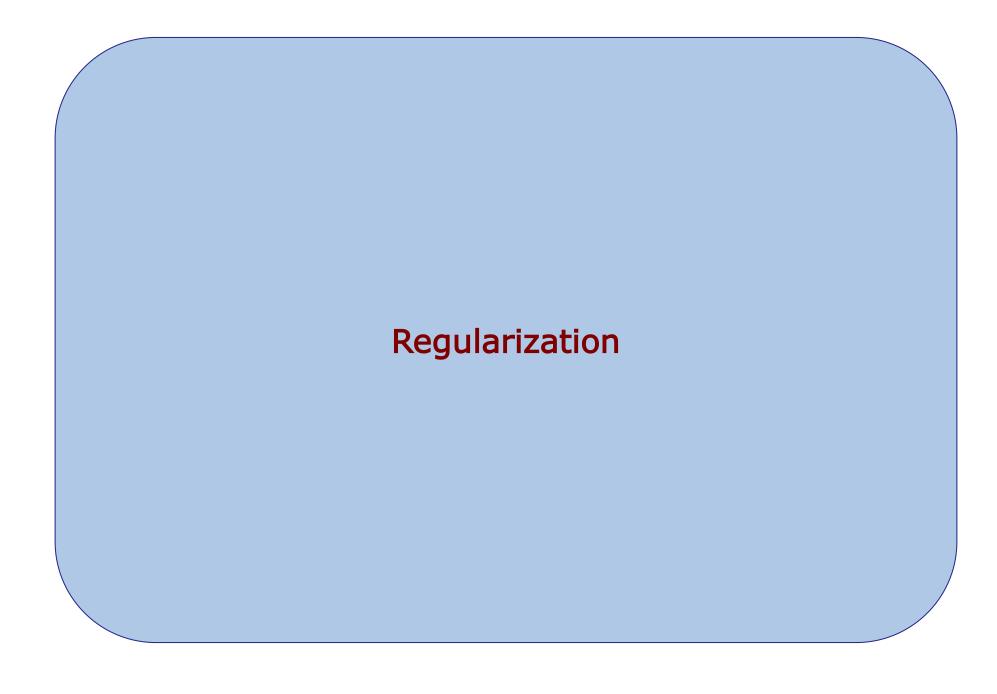
- ☐ What happens if our regression problem has multiple outputs, i.e., t is not scalar
- ☐ It is possible to solve independently a regression problem for each problem
- ☐ Yet, it is possible to use the same set of basis functions:

$$\hat{\mathbf{W}} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{T}$$

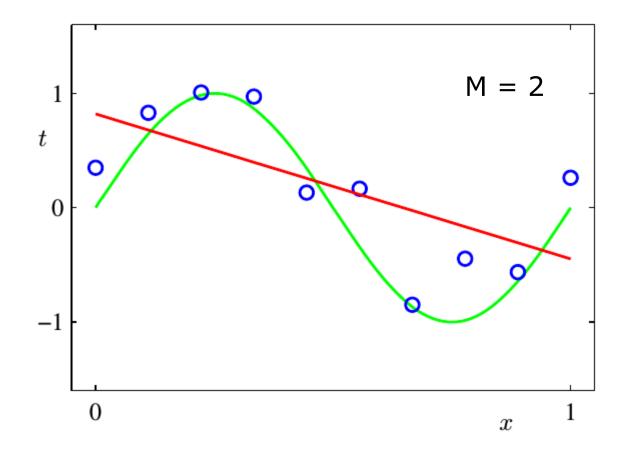
- ▶ Where each column of matrix T and \widehat{W} are respectively the target vector of each and the weight vector for each output
- ☐ The solution above can be easily **decoupled** for each output **k**:

$$\hat{\mathbf{w}}_k = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{t}_k$$

▶ as a benefit $(\Phi^T \Phi)^{-1}$ can be computed only **once**

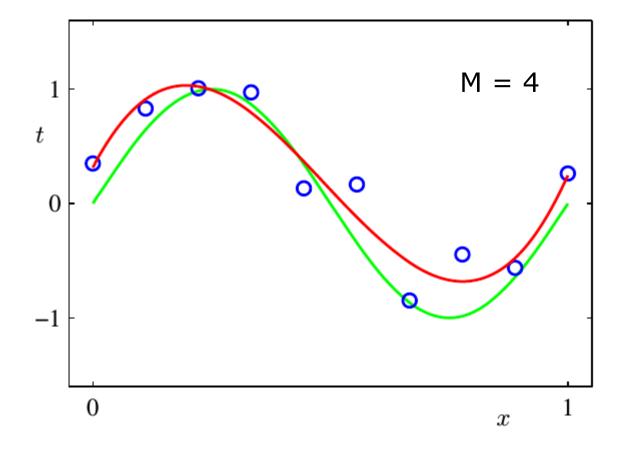


How do we design the linear models? An example



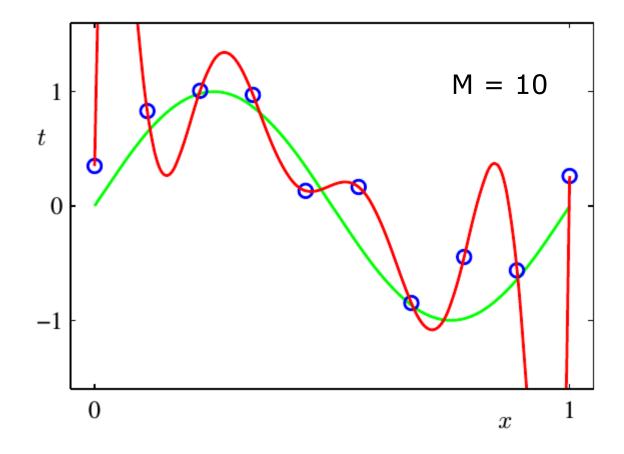
1-order polynomial model

How do we design the linear models? An example



3-order polynomial model

How do we design the linear models? An example



9-order polynomial model

What is regularization?

■ What happens to model parameters when complexity increases?

	M=1	M=2	M = 3	M = 10
\hat{w}_0	0.19	0.82	0.31	0.35
\hat{w}_1		-1.27	7.99	232.37
\hat{w}_2			-25.43	-5321.83
\hat{w}_3				48568.31
\hat{w}_4				-231639.30
\hat{w}_5				640042.26
\hat{w}_6				-1061800.52
\hat{w}_7				1042400.18
\hat{w}_8				-557682.99
\hat{w}_9				125201.43

Regularization

■ How do we extend the loss function?

$$L(\mathbf{w}) = L_D(\mathbf{w}) + \lambda L_W(\mathbf{w})$$

- $\blacktriangleright \mathcal{L}_D(w)$ is the usual loss function (e.g., RSS)
- $\triangleright \mathcal{L}_w(w)$ accounts for model complexity
- $\triangleright \lambda$ is the **regularization** coefficient
- \square How do we design $\mathcal{L}_w(w)$?
 - ► Ridge Regression
 - ► Lasso

Ridge Regression

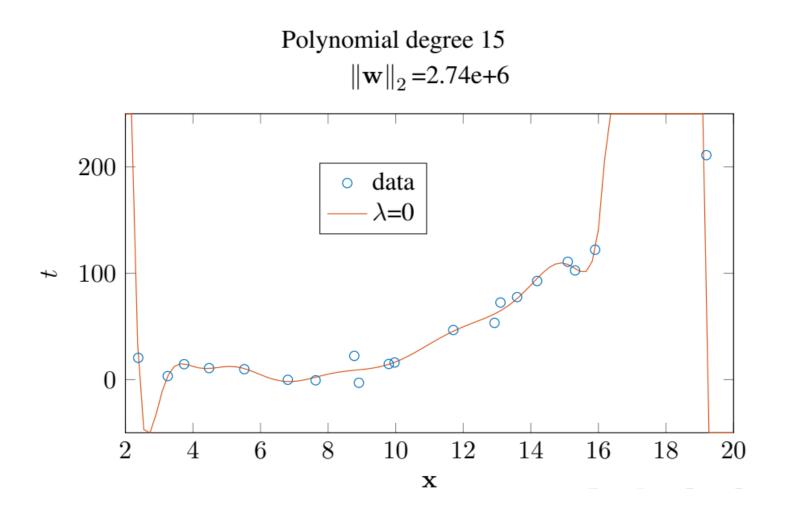
☐ In ridge regression:

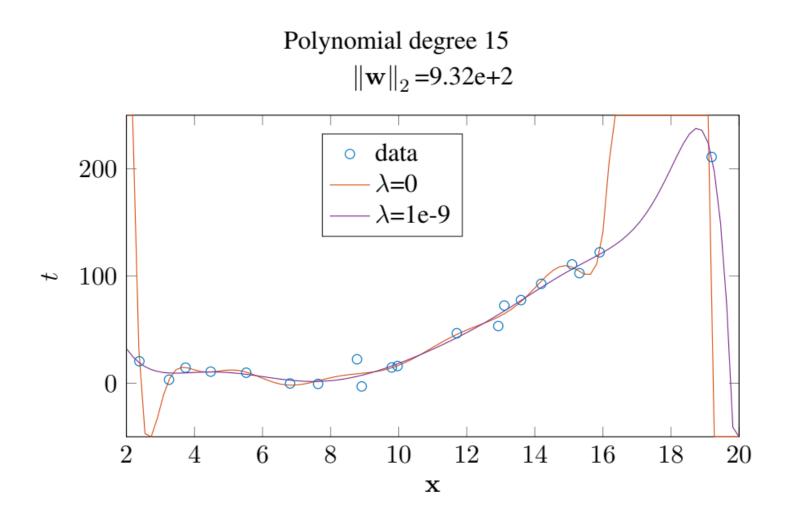
$$L_W(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} = \frac{1}{2} \|\mathbf{w}\|_2^2$$

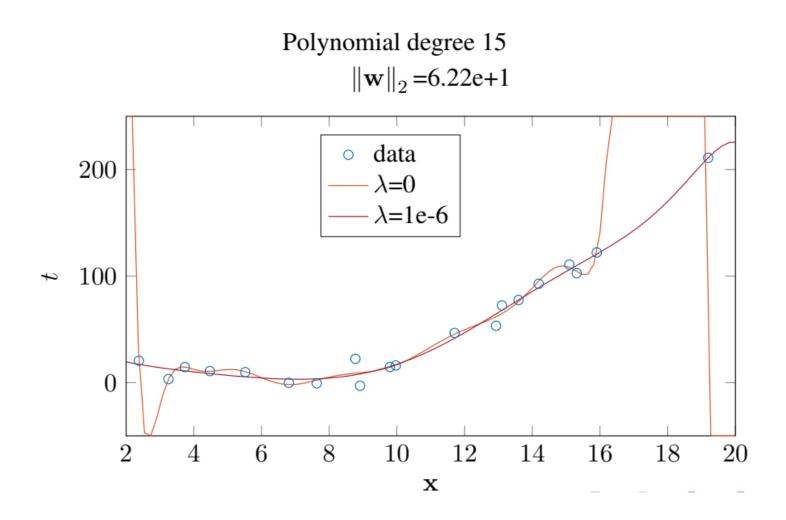
$$L(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} (t_i - \mathbf{w}^T \phi(\mathbf{x}_i))^2 + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

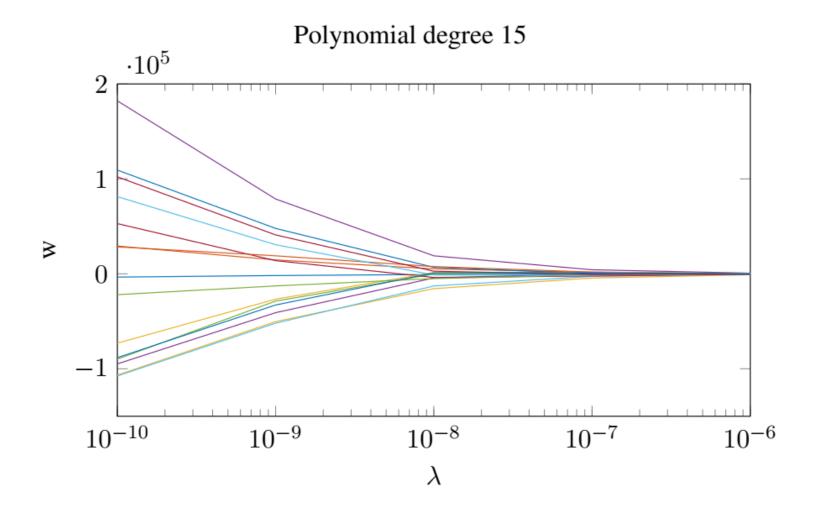
 $lue{}$ The loss function is still quadratic with respect to w and closed-form optimization is still possible:

$$\hat{\mathbf{w}}_{ridge} = \left(\lambda \mathbf{I} + \mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^T \mathbf{t}$$









Lasso

☐ Another common regularization method is **lasso**:

$$L_W(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|_1 = \frac{1}{2} \sum_{j=0}^{M-1} |w_j|$$

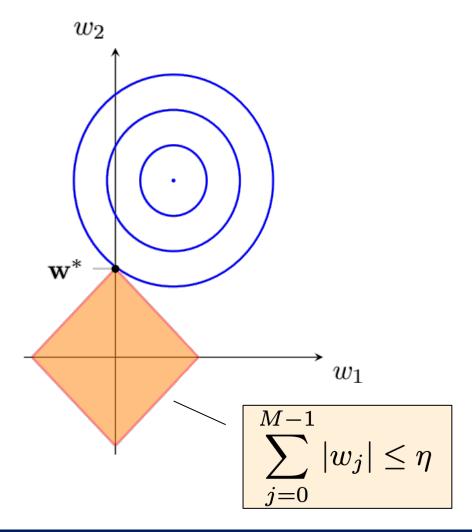
$$L(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} (t_i - \mathbf{w}^T \phi(\mathbf{x}_i))^2 + \frac{\lambda}{2} \|\mathbf{w}\|_1$$

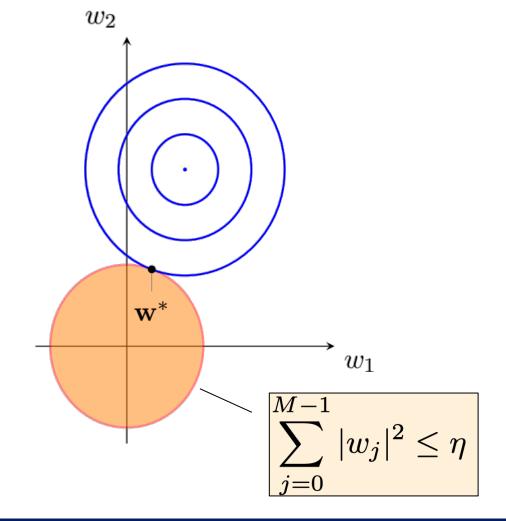
- ☐ In this case, closed-form optimization is not possible
- lacktriangle Nevertheless, lasso typically leads to **sparse** regression models: when regularization coefficient (λ) is large enough, some **components** of \hat{w} become **equal to zero**
- \square We can see regularization equivalent to minimizing $\mathcal{L}_D(w)$ subject to constraint:

$$\sum_{j=0}^{M-1} |w_j| \le \eta$$

Lasso vs Ridge Regression

☐ Why lasso leads to **sparse** model? Let's visualize constraint of lasso and ridge





Least Squares and Maximum Likelihood

Maximum Likelihood (ML)

- ☐ We can deal with regression in a **probabilistic way**
 - ▶ We define a probabilistic model that maps inputs (x) to outputs (t)
 - ▶ Such probabilisic model, y(x, w), will include some **unknown parameters** (w)
 - ▶ Then, we model the **likelihood**, i.e., the probability that observed data \mathcal{D} is generated by a given set of **parameters** (w):

$$p(\mathcal{D}|\mathbf{w})$$

▶ Finally, we can estimate **parameters** (w) by maximizing the likelihood:

$$\mathbf{w}_{ML} = \operatorname*{arg\,max}_{\mathbf{w}} p(\mathcal{D}|\mathbf{w})$$

Maximum Likelihood (ML) for linear regression

☐ Our probabilistic model can be defined as:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^T \phi(\mathbf{x}) + \epsilon$$

- ightharpoonup we assumed a linear model for y(x,w)
- ▶ we assumed $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- □ Given a dataset \mathcal{D} of N samples with inputs $X = \{x_1, ..., x_N\}$ and ouptuts $\mathbf{t} = \{t_1, ..., t_N\}^T$:

$$p(\mathcal{D}|\mathbf{w}) = p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n), \sigma^2\right)$$

Maximum Likelihood (ML) for linear regression (cont.)

 \square To find \mathbf{w}_{ML} it is convenient to maximize the log-likelihood:

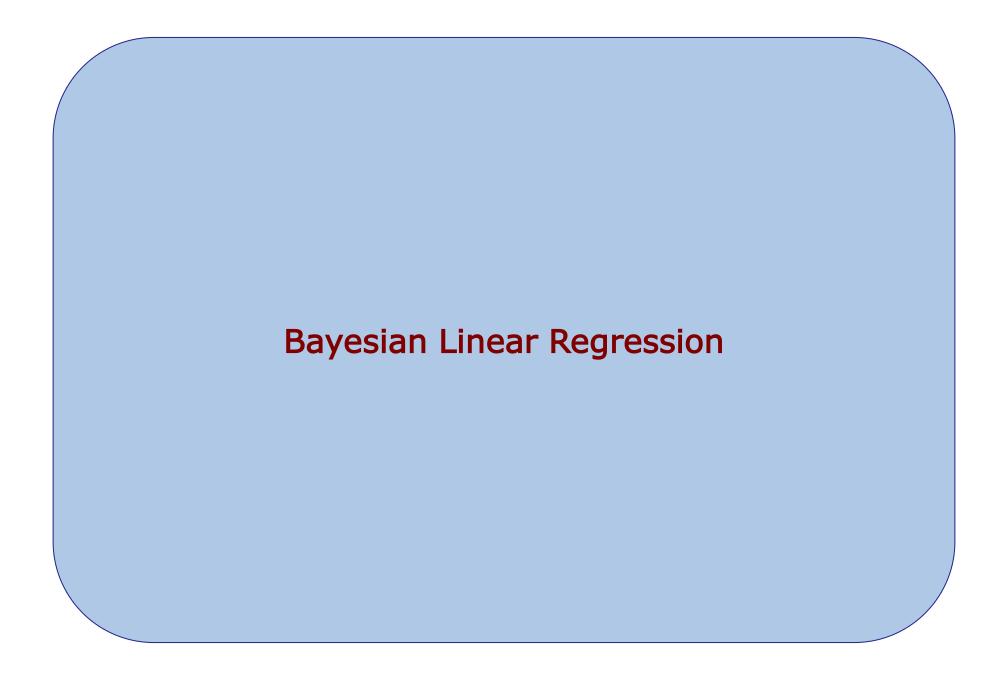
$$\mathcal{N}\left(t_n|\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n), \sigma^2\right) = \frac{1}{(2\pi\sigma^2)^{1/2}} exp\left\{-\frac{1}{2\sigma^2}(t_n - \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n))^2\right\}$$

$$\ell(\mathbf{w}) = \ln p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \sigma^2) = \sum_{n=1}^{N} \ln p(t_n|\mathbf{x}_n, \mathbf{w}, \sigma^2) = -\frac{N}{2} \ln (2\pi\sigma^2) - \frac{1}{2\sigma^2} RSS(\mathbf{w})$$

☐ To solve the optimization problem, we equal the gradient to zero:

$$\nabla \ell(\mathbf{w}) = \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n)^T - \mathbf{w}^T \left(\sum_{n=1}^{N} \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^T \right) = 0$$

$$\Rightarrow \mathbf{w}_{ML} = \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{t}$$
OLS



Bayesian approach

- 1. We formulate our knowledge about the world in a probabilistic way:
 - i. We define the model that expresses our knowledge qualitatively
 - ii. Our model will have some unknown parameters
 - iii. We capture our **assumptions** about unknown parameters with the **prior distribution** over those parameters before seeing the data
- 2. We observe the data
- 3. We compute the posterior probability distribution for the parameters, given observed data

$$p(parameters|data) = \frac{p(data|parameters)p(parameters)}{p(data)}$$

- 4. We use the posterior distribution to:
 - a. Make predictions by averaging over the posterior distribution
 - b. Examine/Account for uncertainty in the parameter values
 - c. Make decisions by minimizing expected posterior loss

☐ The **posterior distribution** for the model parameters can be found by combining the prior with the likelihood for the parameters given data:

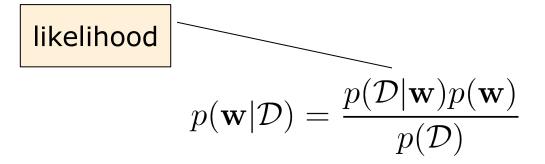
$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

☐ The **posterior distribution** for the model parameters can be found by combining the prior with the likelihood for the parameters given data:

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$
 prior

 $p(\mathbf{w})$ is the **prior** probability over the parameter – what we know before observing the data

☐ The **posterior distribution** for the model parameters can be found by combining the prior with the likelihood for the parameters given data:



▶ $p(D|\mathbf{w})$ is the **likelihood** – the probability of observing the data (D) given some value of the parameters (w)

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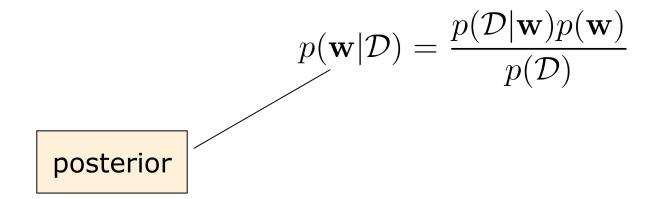
$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

normalizing constant

$$p(\mathcal{D}) = \int p(\mathcal{D}|\mathbf{w})p(\mathbf{w})d\mathbf{w}$$

ightharpoonup P(D) is the marginal likelihood and acts as normalizing constant

☐ The **posterior distribution** for the model parameters can be found by combining the prior with the likelihood for the parameters given data:



- $ightharpoonup p(\mathbf{w}|D)$ is the **posterior probability** of parameters w given training data
- ▶ the most probable value of w given the data will be the mode of the posterior, also known as maximum a posteriori (MAP).

Bayesian Linear Regression

☐ How to model the **prior**? Assuming a Gaussian likelihood, a **conjugate prior** is the most convenient choice:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{S}_0)$$

Bayesian Linear Regression

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$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{S}_0)$$

☐ As a result, the **posterior** is still Gaussian:

$$p(\mathbf{w}|\mathbf{t}, \mathbf{\Phi}, \sigma^2) \propto \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{S}_0) \mathcal{N}(\mathbf{t}|\mathbf{\Phi}\mathbf{w}, \sigma^2\mathbf{I})$$

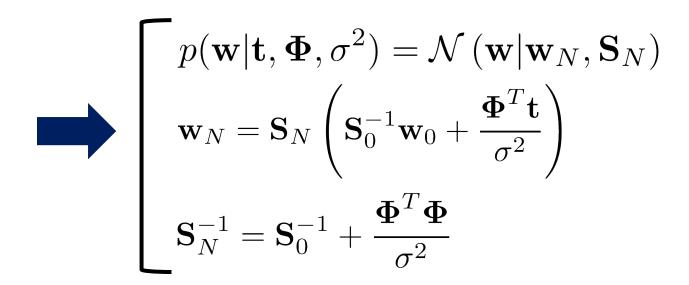
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Bayesian Linear Regression an Maximum Likelihood

- Which parameters?
 - ▶ The maximum a-posteriori (MAP) is the obvious choice
 - ▶ When posterior is gaussian the MAP is equal to the mean
- ☐ When prior is **infinitely broad** MAP is equal to ML solution:

$$\lim_{\mathbf{S}_0 \to \infty} \mathbf{w}_N = \left(\mathbf{\Phi}^T \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^T \mathbf{t}$$

$$\lim_{\mathbf{S}_0 \to \infty} \mathbf{S}_N^{-1} = \frac{\mathbf{\Phi}^T \mathbf{\Phi}}{\sigma^2}$$

$$\hat{\sigma^2} = \frac{1}{N - M} \sum_{n=1}^{N} (t_n - \hat{\mathbf{w}}^T \boldsymbol{\phi}(\mathbf{x}_n))^2$$

► The ML estimate of w has the smallest variance among linear unbiased estimates and the lowest MSE among linear unbiased estimates (Gauss-Markov).

Bayesian Linear Regression and Regularization

- What about regularization?
 - ▶ When $\mathbf{w}_0 = 0$ and $\mathbf{S}_0 = \tau^2 \mathbf{I}$, we have:

$$\ln p(\mathbf{w}|\mathbf{t}) = -\frac{1}{2\sigma^2} \sum_{i=1}^{N} \left(t_i - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) \right)^2 - \frac{1}{2\tau^2} \|\mathbf{w}\|_2^2$$

▶ In this case, MAP (\mathbf{w}_N) is equivalent to the solution of ridge regression ($\widehat{\mathbf{w}}_{ridge}$) with $\lambda = \frac{\sigma^2}{\tau^2}$

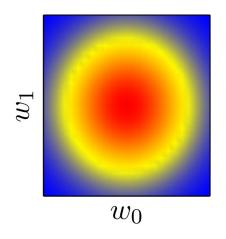
Machine Learning

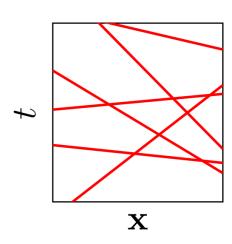
Bayesian Linear Regression: an example

- ☐ How to exploit the Bayesian approach for sequential learning?
 - ► We compute **posterior** with initial data
 - When additional data is available, the posterior becomes the prior

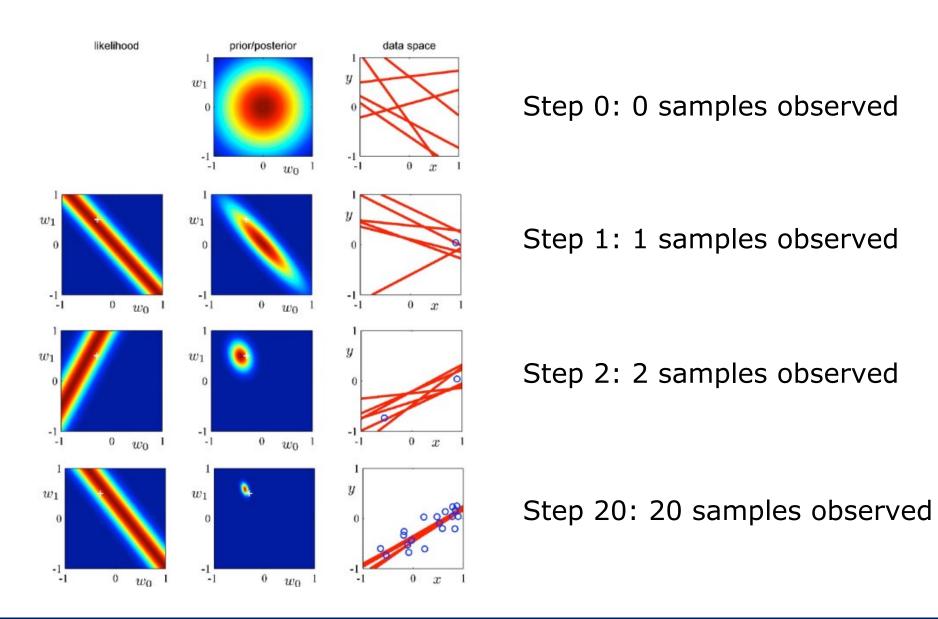
Bayesian Linear Regression: an example

- How to exploit the Bayesian approach for sequential learning?
 - ▶ We compute **posterior** with initial data
 - When additional data is available, the posterior becomes the prior
- ☐ Let see an example
 - ▶ Let assume data is generated as $t(x) = -0.3 + 0.5x + \varepsilon$
 - ▶ Let assume that $x \sim U(-1,1)$ and $\varepsilon \sim \mathcal{N}(0,0.04)$
 - ▶ Let use as model: $y(x, \mathbf{w}) = w_0 + w_1 x$
 - ▶ Let assume as prior: $p(\mathbf{w}) = \mathcal{N}(\mathbf{w_0}, \tau^2 \mathbf{I})$ with $\tau^2 = 0.5$ and $\mathbf{w_0} = [0,0]^T$





Bayesian Linear Regression: an example (2)



Predictive Distribution

 \square With a Bayesian framework, it is possible to compute the probability distribution of the target for a new sample \mathbf{x}^* (given the training data \mathcal{D}), by integrating over the posterior distribution:

$$p(t^*|\mathbf{x}^*, \mathcal{D}) = \mathbb{E}[t^*|\mathbf{x}^*, \mathbf{w}, \mathcal{D})] = \int p(t^*|\mathbf{x}^*, \mathbf{w}, \mathcal{D})p(\mathbf{w}|\mathcal{D})d\mathbf{w}$$

- ☐ This is often called **predictive distribution**
- Unfortunately, computing the predictive distribution requires knowledge of the posterior distribution, which is usually intractable

Predictive Distribution for Bayesian Regression

☐ With our assumptions, we can compute the **predictive distribution**:

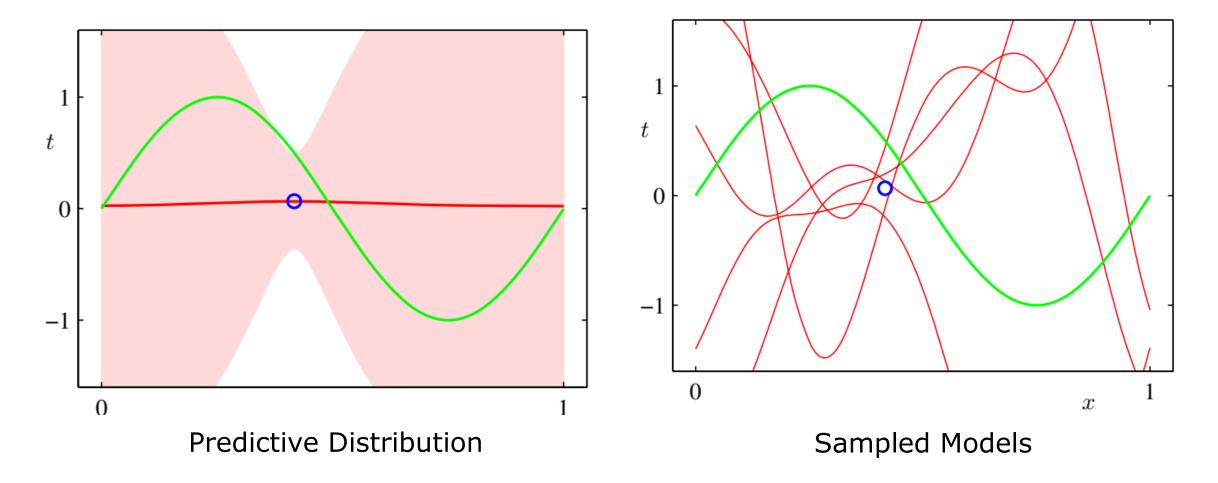
$$p(t|\mathbf{x}, \mathcal{D}, \sigma^2) = \int p(t|\mathbf{x}, \mathbf{w}, \sigma^2) p(\mathbf{w}|\mathbf{w}_N, \mathbf{S}_N) d\mathbf{w} = \int \mathcal{N}(t|\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}), \sigma^2) \mathcal{N}(\mathbf{w}|\mathbf{w}_N, \mathbf{S}_N) d\mathbf{w}$$
$$p(t|\mathbf{x}, \mathcal{D}, \sigma^2) = \mathcal{N}(t|\mathbf{w}_N^T \boldsymbol{\phi}(\mathbf{x}), \sigma_N^2(\mathbf{x}))$$

$$\sigma_N^2(\mathbf{x}) = \sigma^2 + \phi(\mathbf{x})^T \mathbf{S}_N \phi(\mathbf{x})$$

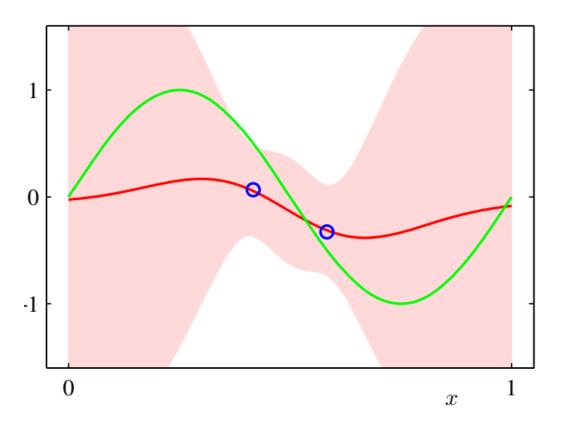
$$\frac{\text{data}}{\text{parameters}}$$

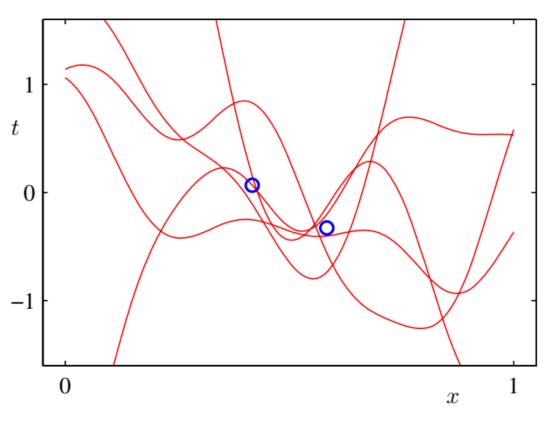
▶ when $N \to \infty$ the uncertainty associated to parameters (second term) goes to zero and the variance of predictive distribution depends only on variance of data (σ^2)

□ Approximating a sinusoidal dataset with a linear model w/ 9 Gaussian basis functions: 1 sample observed



□ Approximating a sinusoidal dataset with a linear model w/ 9 Gaussian basis functions: 2 samples observed

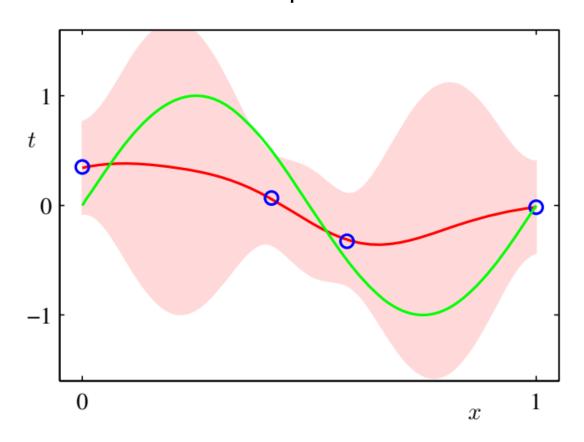


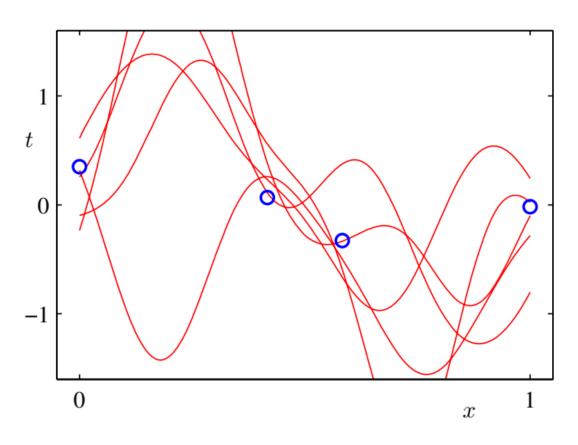


Predictive Distribution

Sampled Models

□ Approximating a sinusoidal dataset with a linear model w/ 9 Gaussian basis functions: 4 samples observed

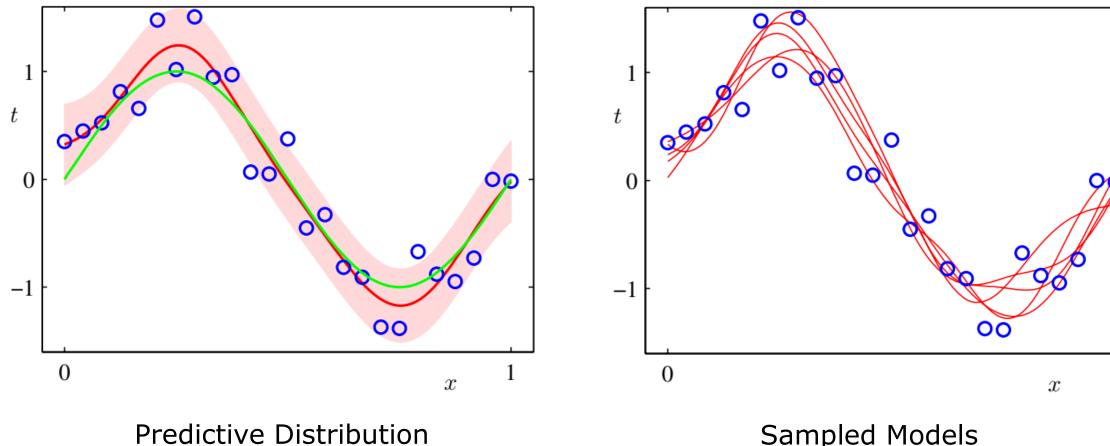




Predictive Distribution

Sampled Models

□ Approximating a sinusoidal dataset with a linear model w/ 9 Gaussian basis functions: 25 samples observed



Sampled Models

Challenges and Limitation of Linear Regression

Challenges

- Modeling Challenges
 - ► Our model should fit well all the functions (we think) are likely
 - ► The prior should not give zero or small probabilities to possible values, but at the same time also avoid spreading out the probability (uninformative)
- Computational Challenges
 - Analytical integreation is possible only using conjugate priors and works for simple models
 - ► Approximated approaches are instead to be used in the more general case, such as Gaussian (Laplace) approximation, Monte Carlo integration, and Variational approximation

Limitation of Fixed Basis Functions

- ☐ Linear models with fixed basis functions have several advantages
 - Allow closed-form solution
 - ► Tractable **Bayesian treatment**
 - Can model non-linear relationship with proper basis function
- ☐ However, they have also several limitations
 - Basis functions are not adaptive with respect to the training data
 - ▶ These models suffer of the curse of dimensionality