Linear Regression

Machine Learning

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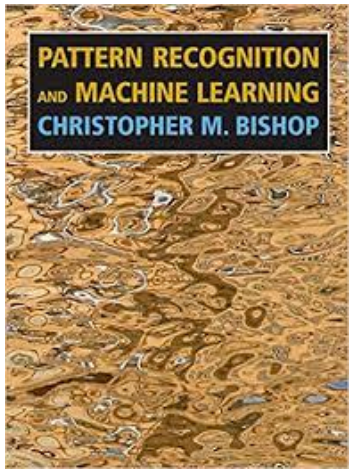
POLITECNICO
MILANO 1863

References

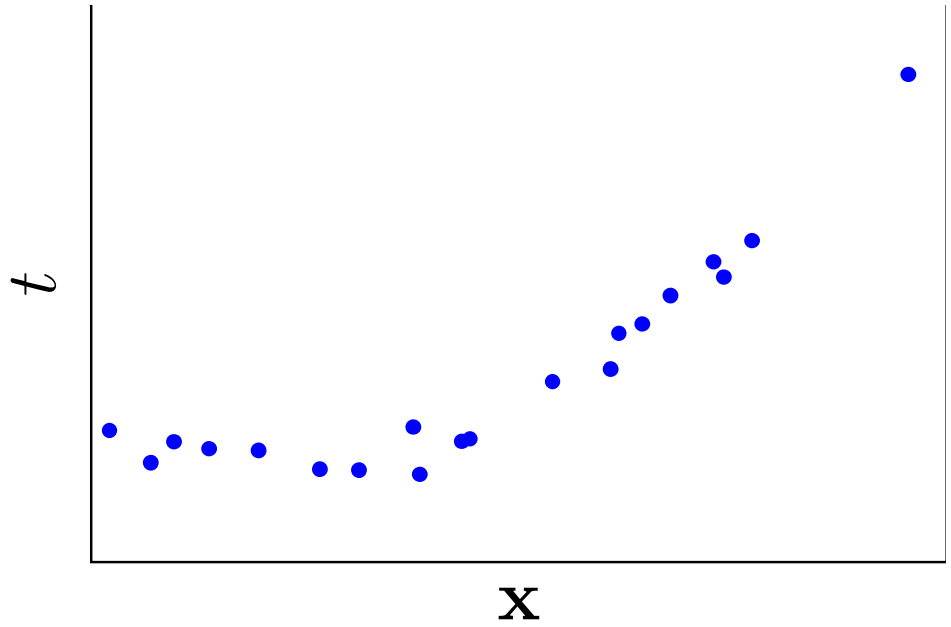
- *Pattern Recognition and Machine Learning*, Bishop
  - Chapter 1 (1.1, 1.2, 1.3)
  - Chapter 3 (3.1, 3.3)



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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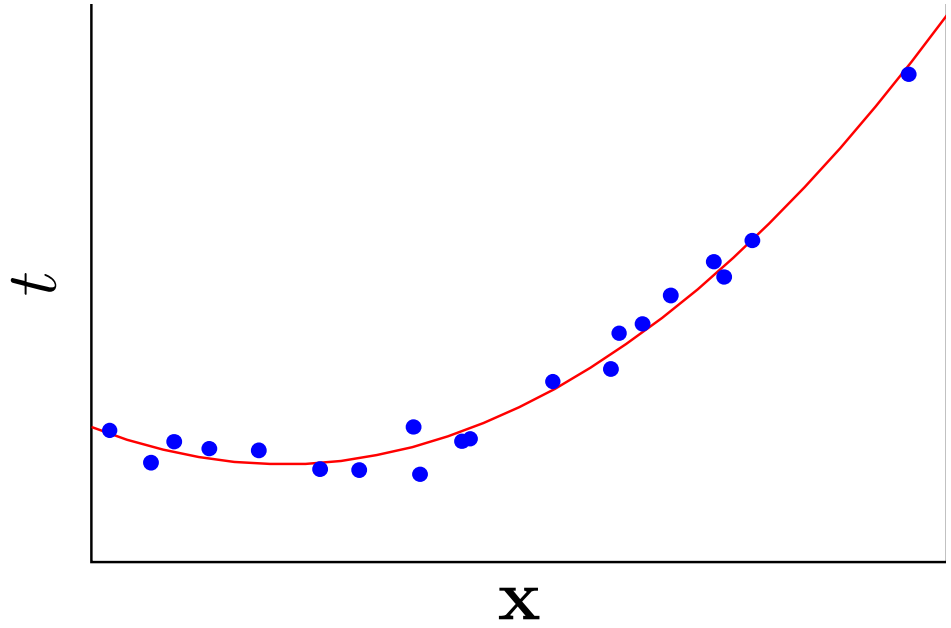
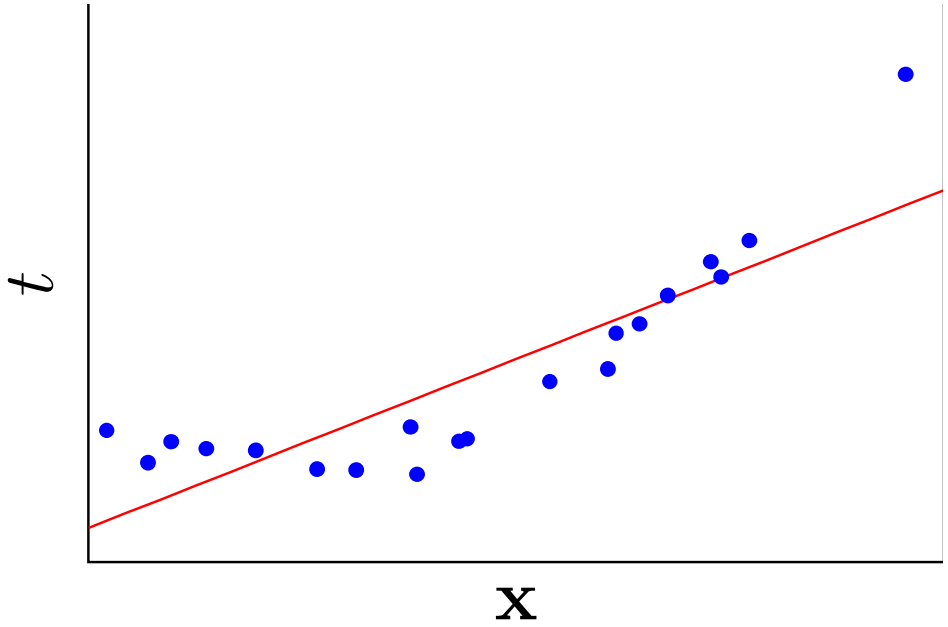
  - How do we model f?
  - How do we evaluate our approximation?
  - How do we optimize our approximation?



Linear Regression

- 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

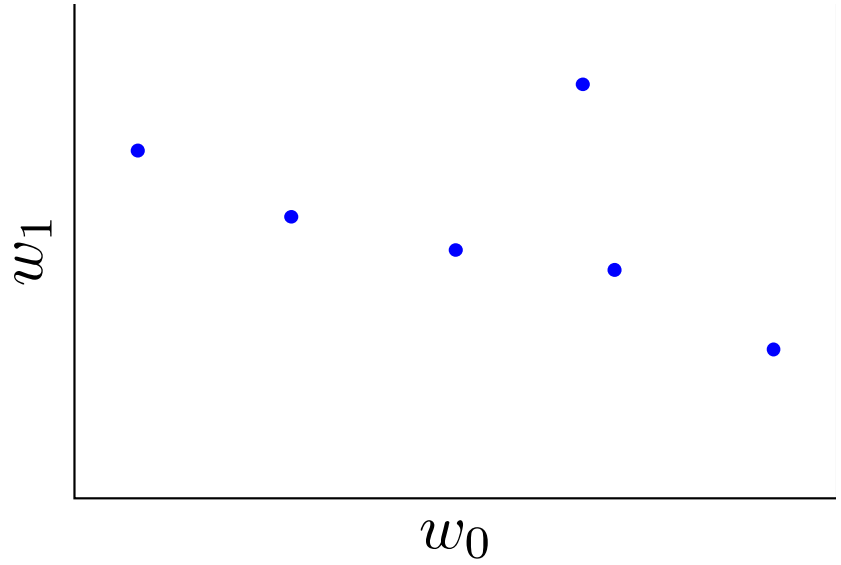


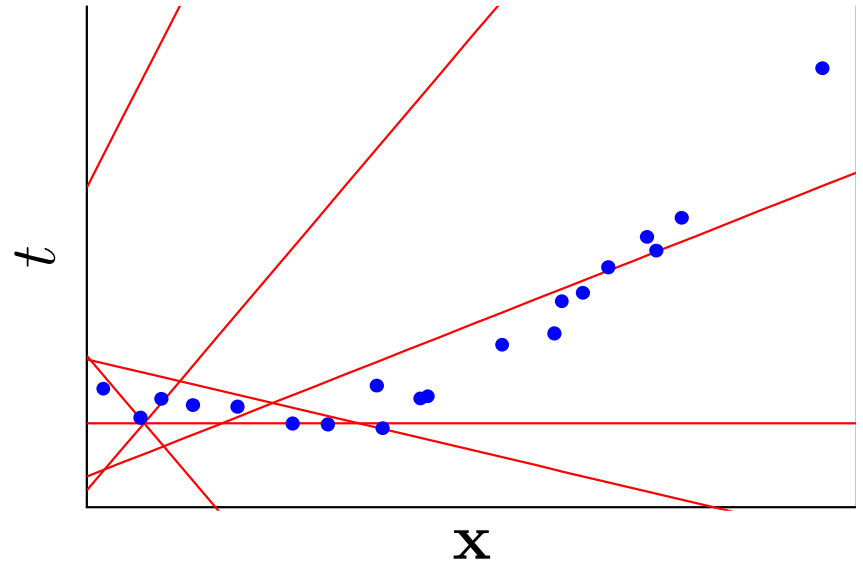
Linear Regression: model

- The simplest linear model can be defined as:

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

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





Linear Regression: loss function and optimization

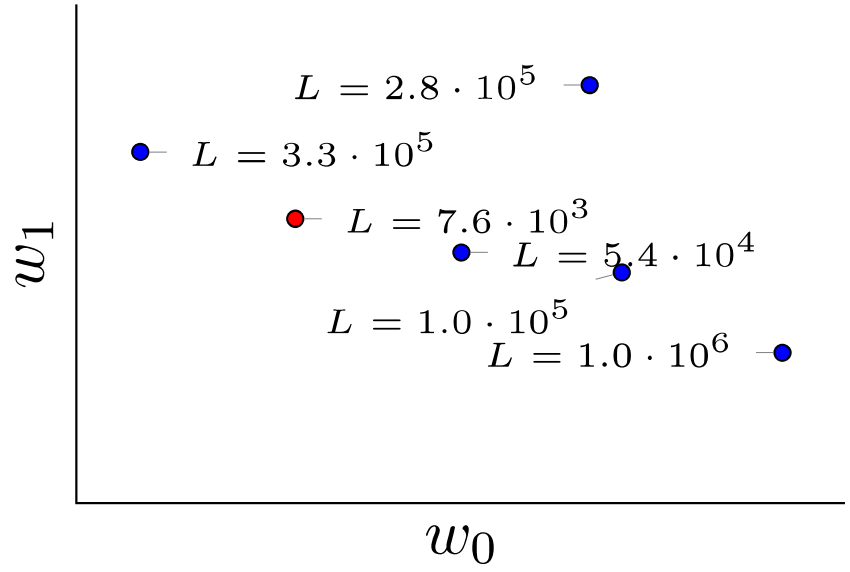
- A convenient **error loss function** is the **sum of squared errors** (SSE):

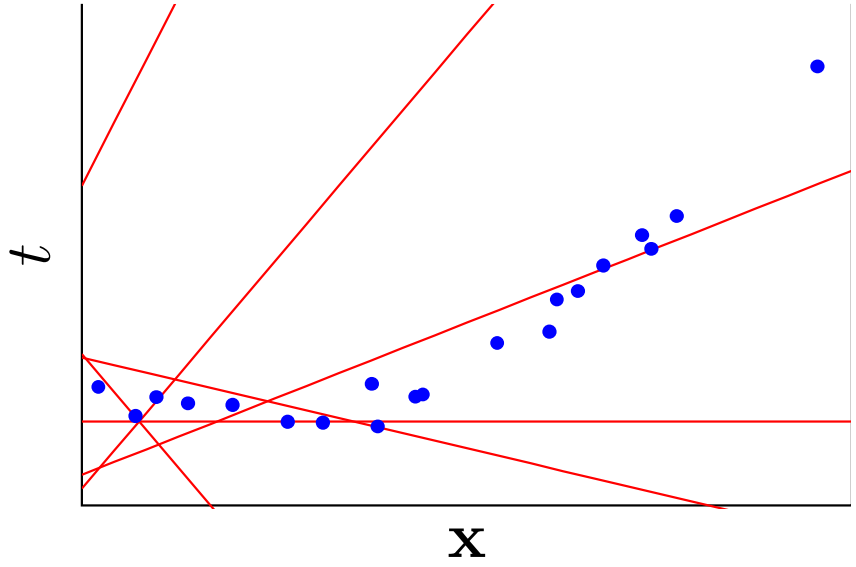
$$L(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(y(x_n, \mathbf{w}) - t_n\right)^2$$

  - the sum in $\mathcal{L}$ 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 $\mathcal{L}$ can be easily obtained





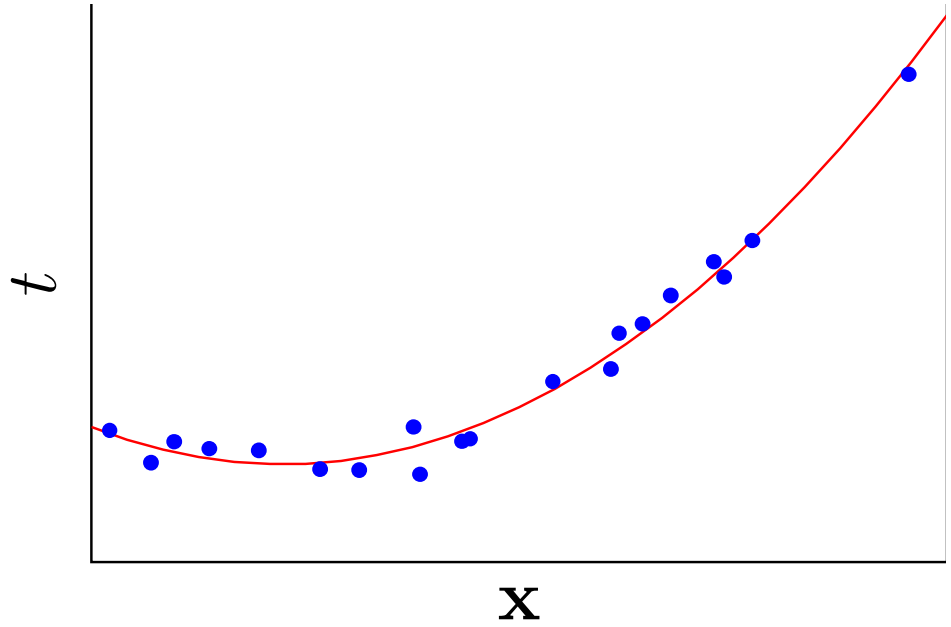
Linear Models and Basis Functions

Linear Models

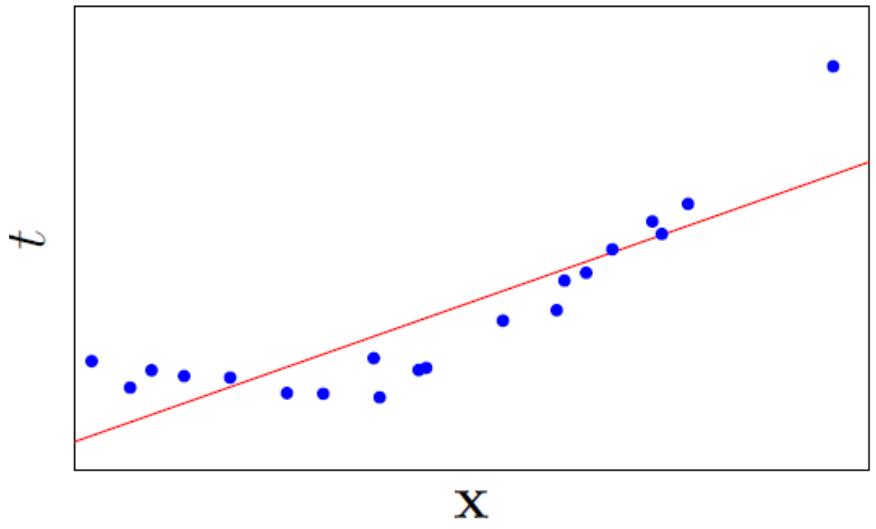
- A linear combination of the input variables is not enough to model data…
- … but we just need a regression model that is **linear in the parameters**
- We can define a model using non-linear **basis functions**:

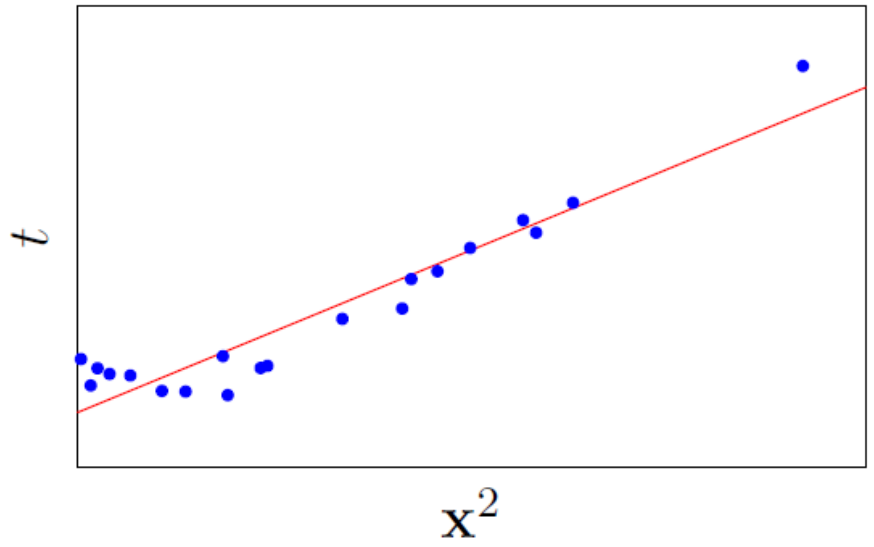
$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})$$

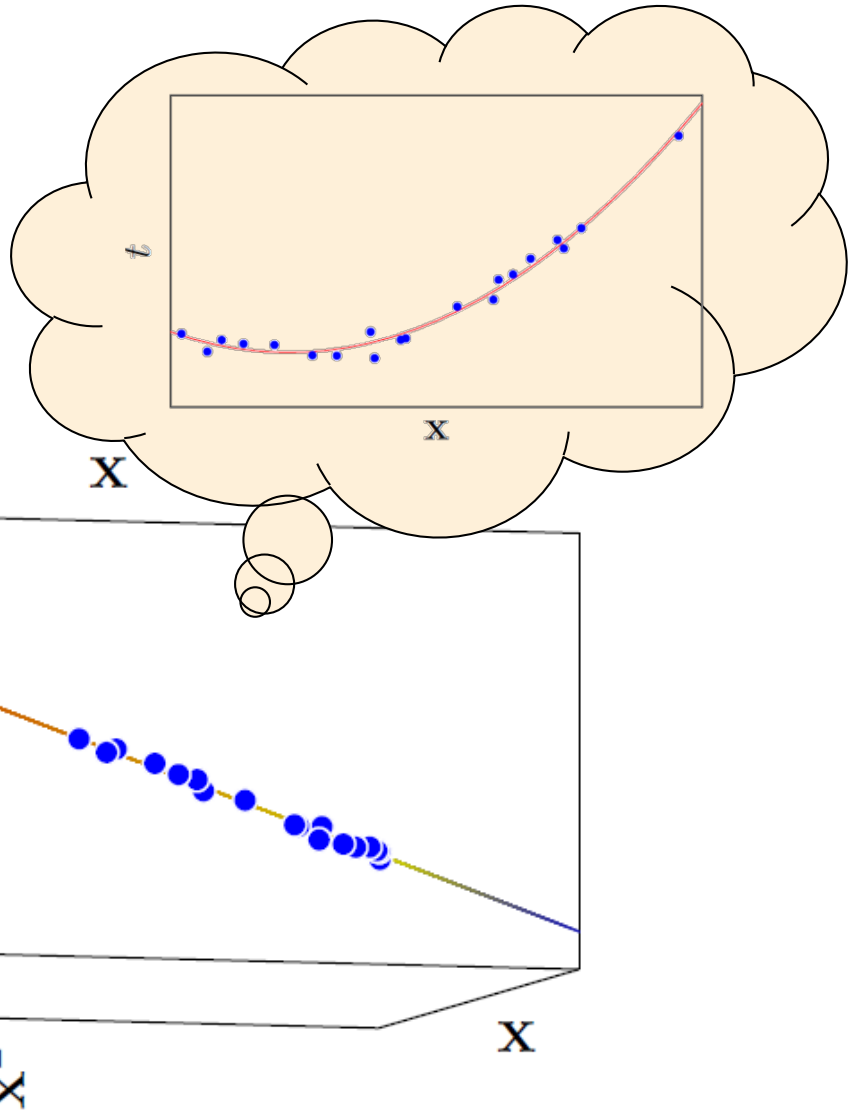
  - $\boldsymbol{\phi}(\mathbf{x}) = (1, \phi_1(\mathbf{x}), \ldots, \phi_{M-1}(\mathbf{x}))^T$



Let see it in feature space…



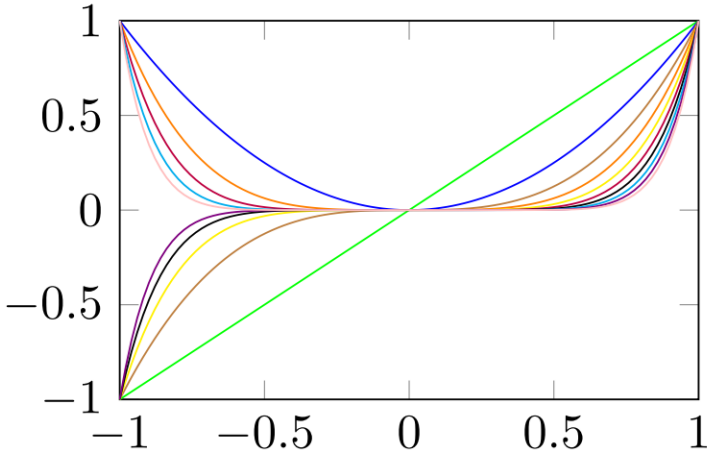




Basis Functions

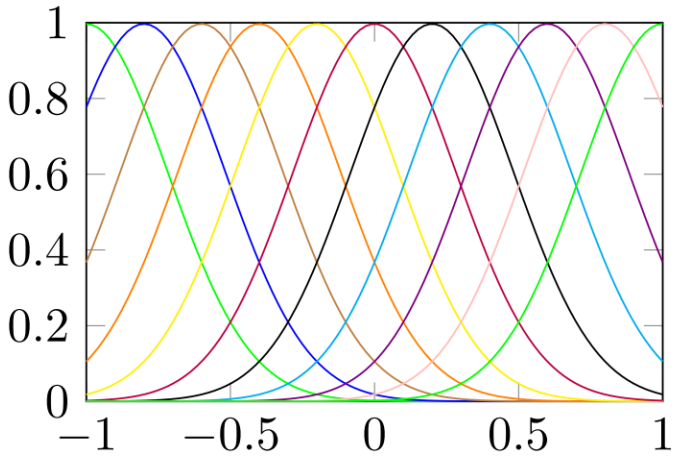
- Some examples of basis function (assuming single-variable input)

Polynomial



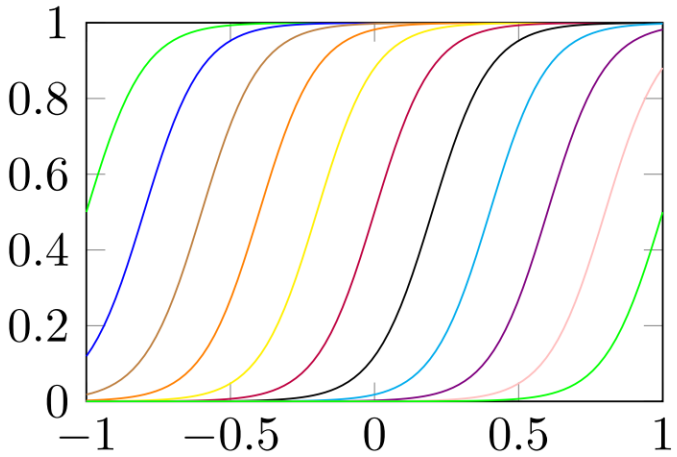
$$\phi_j(x) = x^j$$

Gaussian



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

Sigmoidal



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

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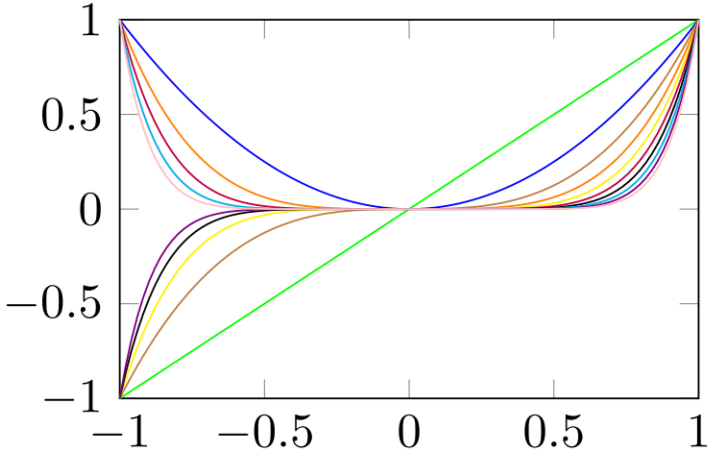

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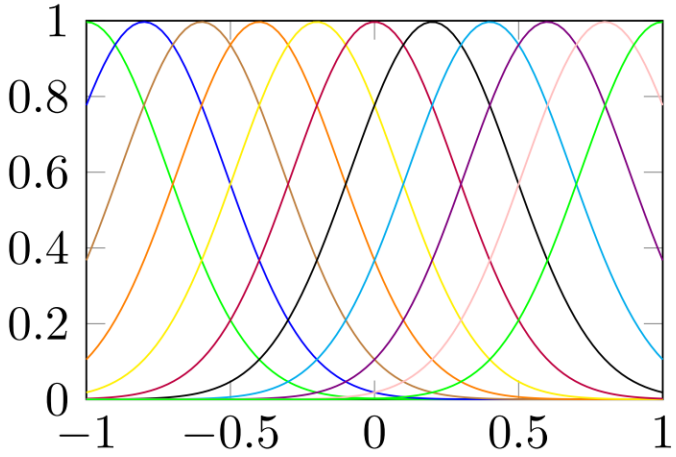

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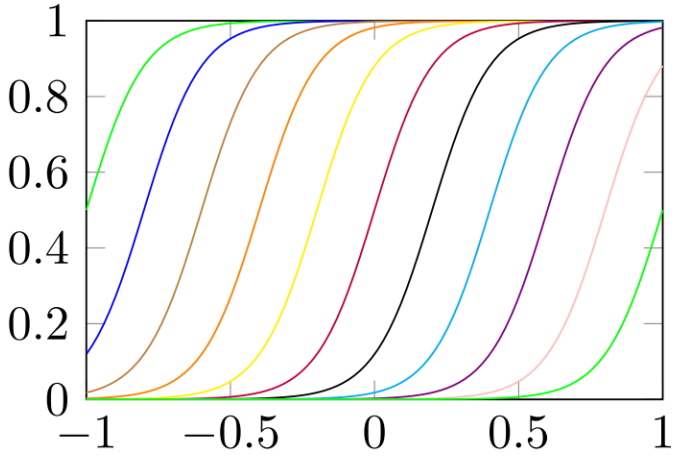
LOCAL

Sigmoidal



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Least Squares

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:

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

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

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

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

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

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Assuming ($\boldsymbol{\Phi}^T \boldsymbol{\Phi}$) non singular
Complexity $O(NM^2 + M^3)$

Sequential Learning

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

$$L(\mathbf{x}) = \sum_n L(x_n)$$

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

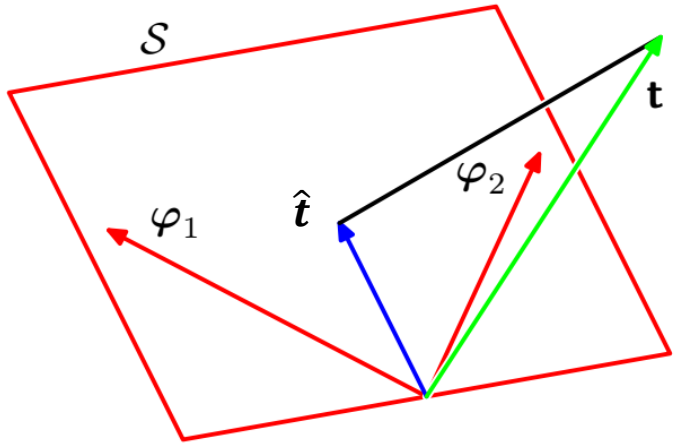
$$\Rightarrow \mathbf{w}^{(n+1)} = \mathbf{w}^{(n)} - \alpha^{(n)} \left(\mathbf{w}^{(n)^T} \boldsymbol{\phi}(\mathbf{x}_n) - t_n \right) \boldsymbol{\phi}(\mathbf{x}_n)$$

- α is called learning rate and to guarantee convergence:

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

Geometric Interpreation of OLS

- Let $\boldsymbol{t}$ be the N-dimensional target vector
- Let φ_j be the j-th column of matrix $\boldsymbol{\Phi}$
  - $\varphi_1, \ldots, \varphi_M$ identify a linear subspace $\mathcal{S}$
- Let $\hat{\boldsymbol{t}}$ be the N-dimensional vector computed as $\boldsymbol{\Phi w}$
  - $\hat{\boldsymbol{t}}$ is a linear combination of φ_j and lies in $\mathcal{S}$
- OLS finds $\hat{\boldsymbol{t}}$ minimizing the SSE with respect to $\boldsymbol{t}$
  - $\hat{\boldsymbol{t}}$ represents the projection of $\boldsymbol{t}$ onto the subspace $\mathcal{S}$



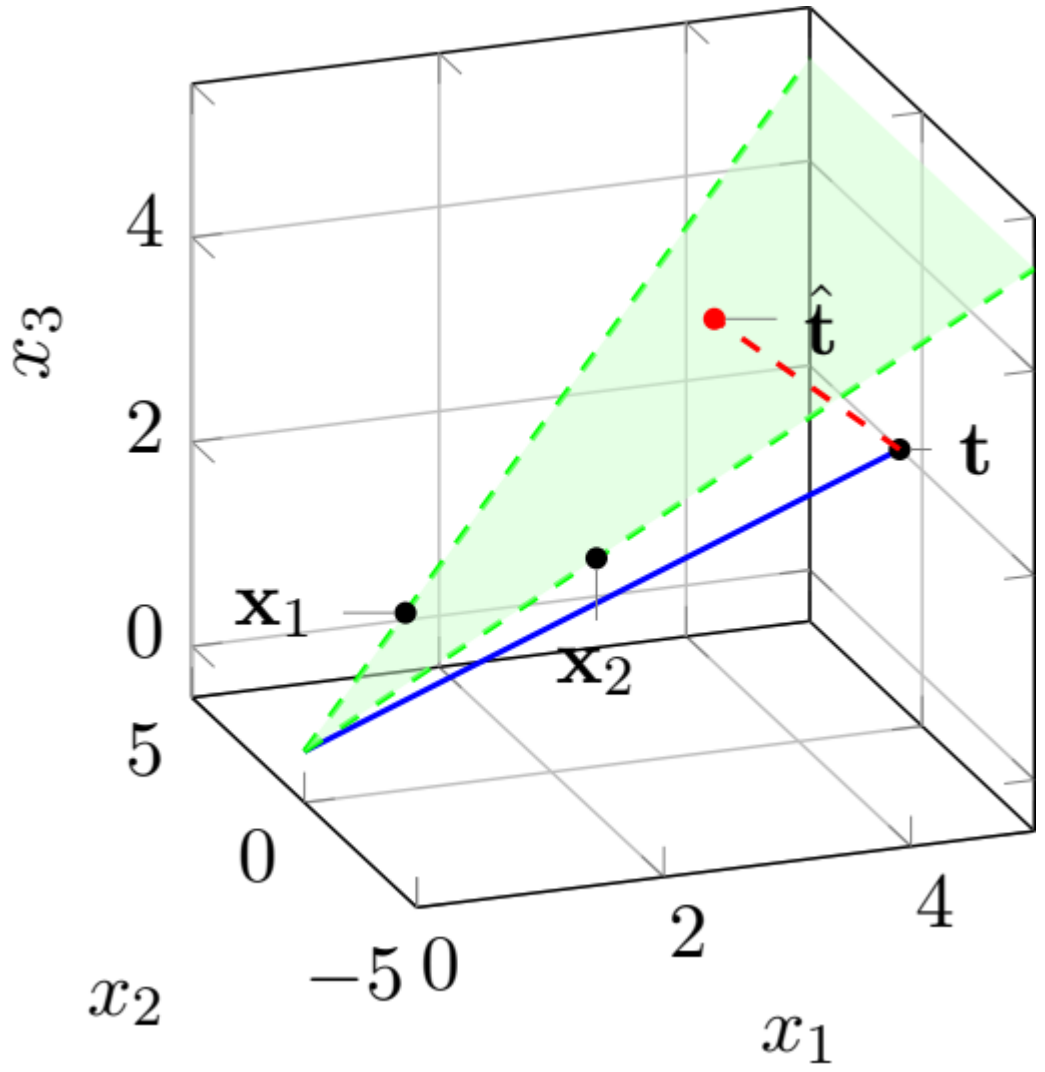
$$\hat{\mathbf{t}} = \boldsymbol{\Phi}\hat{\mathbf{w}} = \underbrace{\boldsymbol{\Phi}\left(\boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T}_{\text{Hat Matrix (H)}}\mathbf{t}$$

Geometric Interpreation of OLS: an example

- 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 $\hat{W}$ 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**:

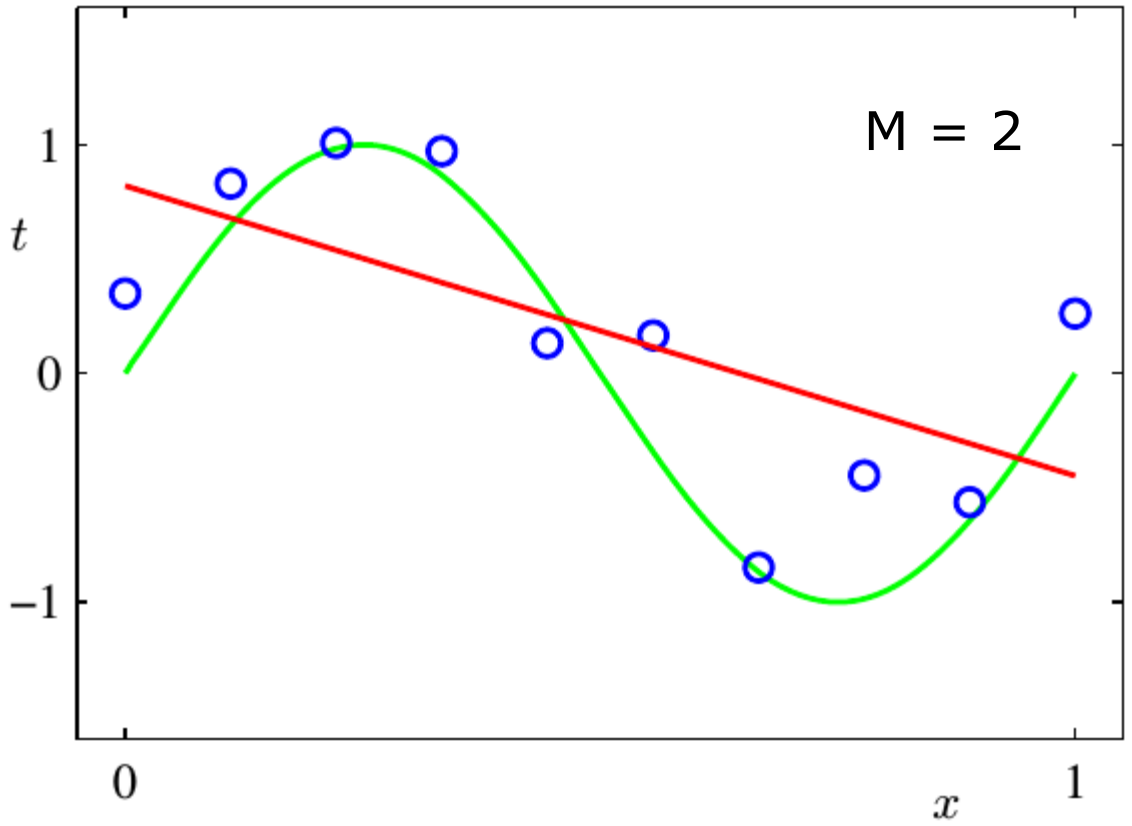
$$\hat{\mathbf{w}}_k = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{t}_k$$

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

Regularization

How do we design the linear models? An example

$y = w_0 + w_1 x$ ⇝ clearly it's not a good model ...

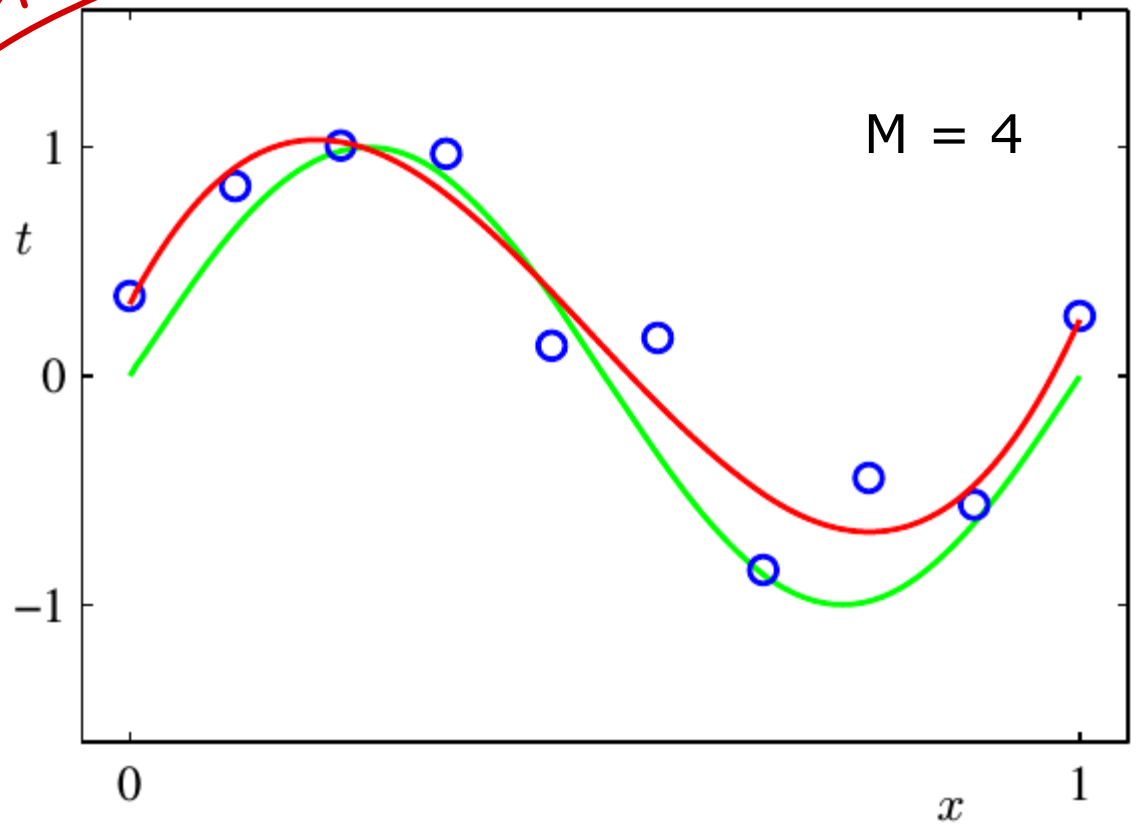


1-order polynomial model

How do we design the linear models? An example

$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$ → it seems better.

I add new features.

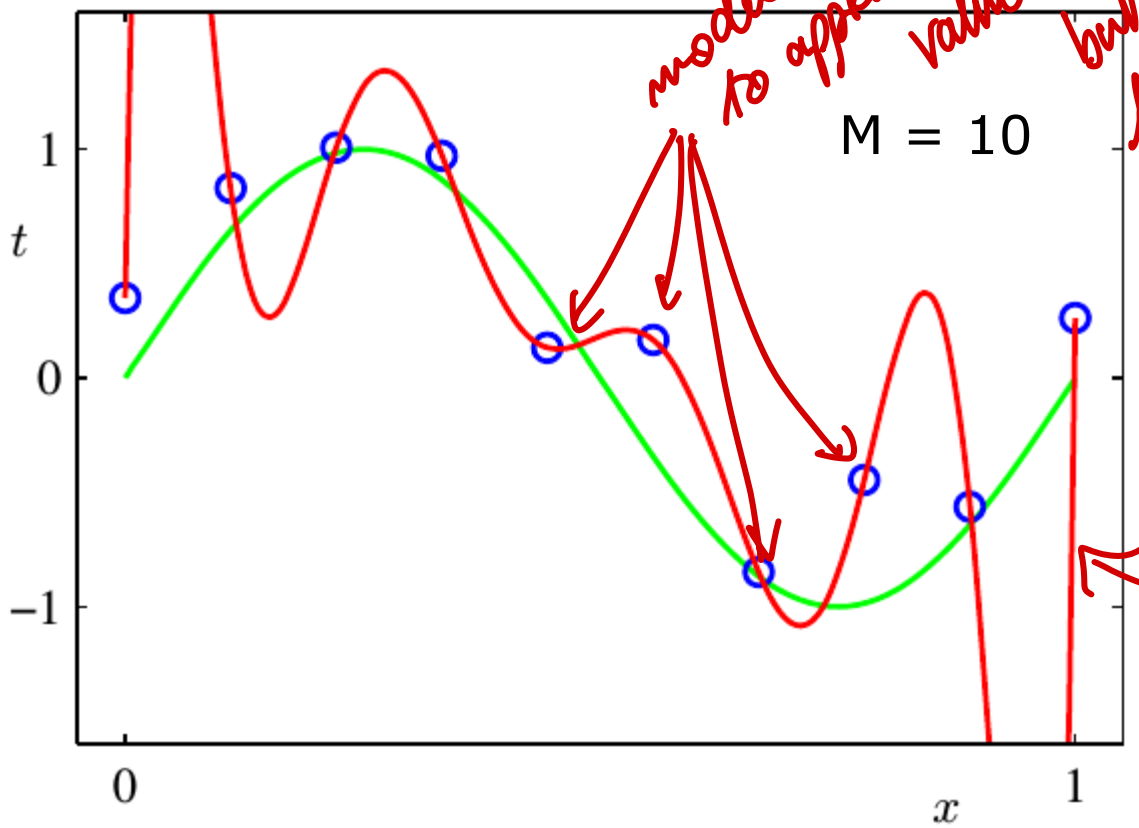


$$\phi(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \end{bmatrix}$$

3-order polynomial model

↳ I might use higher degrees... but when to stop??

How do we design the linear models? An example



model is really good to approximate the target value in each data point but very bad to approx. the green curve!

"Overfitting"

This is definetely not a good solution!

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

quite small weights: OK!

we don't want so large weights !!

The more I increase the order, the larger weight values ...

... model has to change dramatically the value @ each data point.

Regularization

- How do we extend the loss function?

$$L(\mathbf{w}) = \overbrace{L_D(\mathbf{w})}^{\text{RSS}} + \lambda L_W(\mathbf{w})$$

This part of the loss is here to penalize solutions with weight vector which is large (large weights).

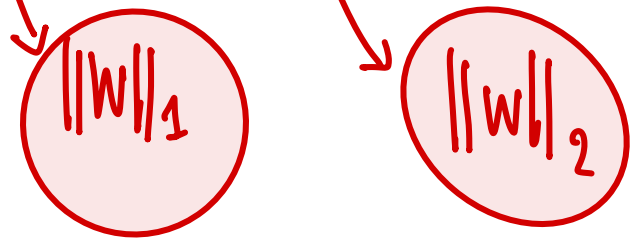
"smooth"

  - $\mathcal{L}_D(w)$ is the usual loss function (e.g., RSS)
  - $\mathcal{L}_w(w)$ accounts for model complexity
  - λ is the **regularization** coefficient

has to be fitted to find a good tradeoff between "performance" & "model complexity".

- How do we design $\mathcal{L}_w(w)$?
  - Ridge Regression
  - Lasso

most used $\mathcal{L}_w(w)$.



1) Ridge Regression → $\|w\|_2$

- In **ridge regression**:

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

$$\Rightarrow \quad L(\mathbf{w}) = \underbrace{\frac{1}{2}\sum_{i=1}^{N}\left(t_i - \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i)\right)^2}_{\text{RSS}} + \underbrace{\frac{\lambda}{2}\|\mathbf{w}\|_2^2}_{\lambda L_W(w)}$$

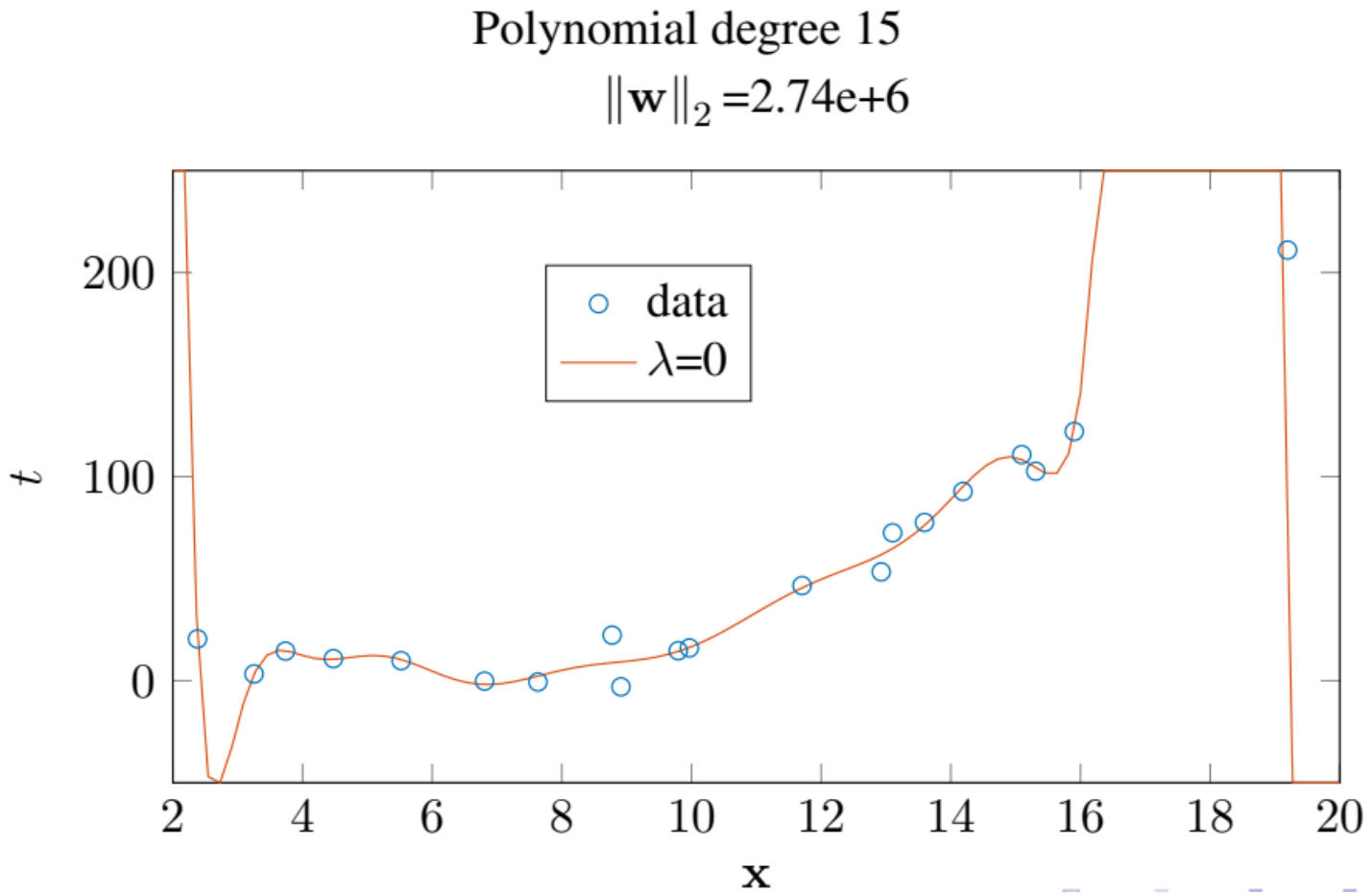
- The loss function is still quadratic with respect to w and closed-form optimization is still possible:

benefit: guarantee that the matrix is invertible thanks to the λI term.
↳ can be used even if two features are linearly dependent.

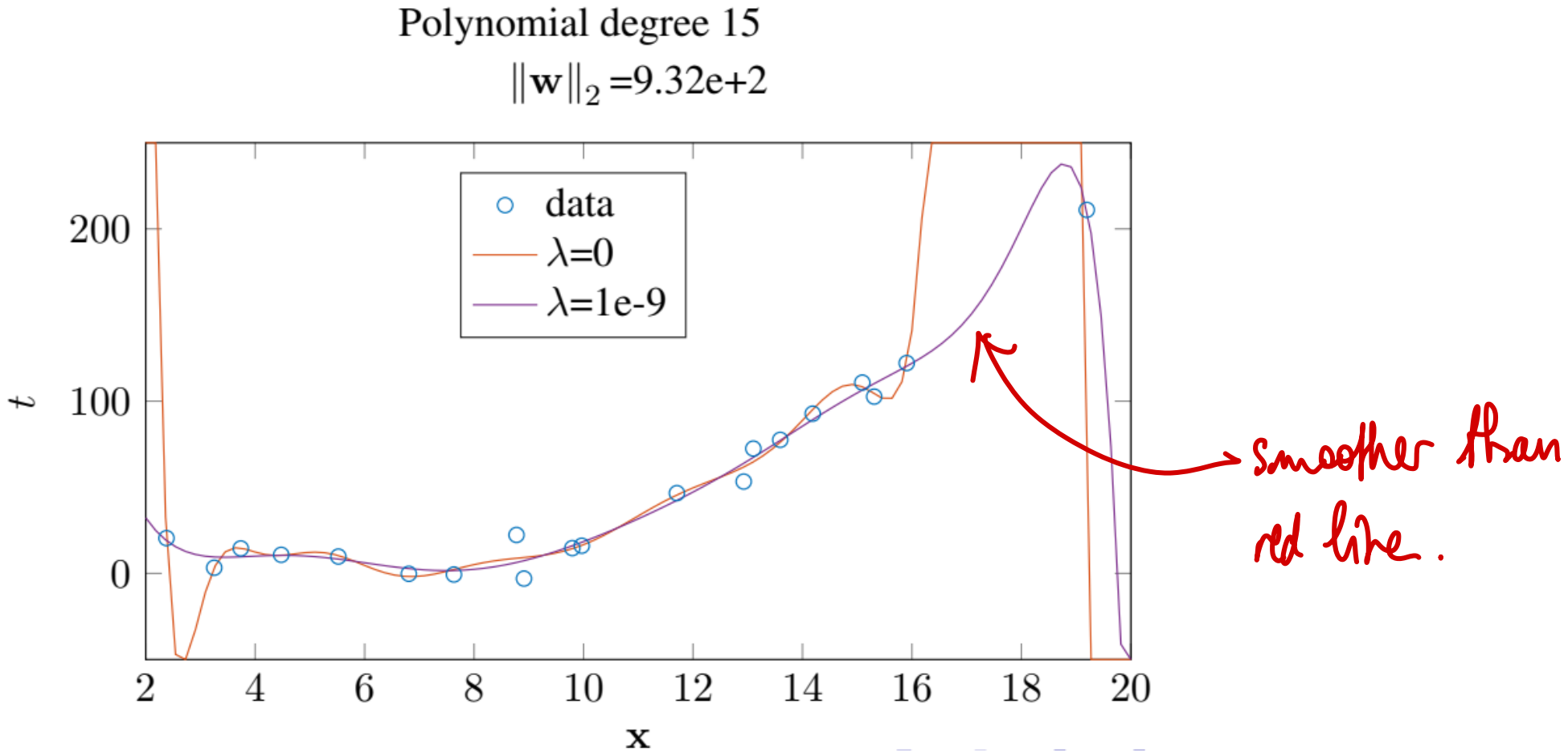
$$\hat{\mathbf{w}}_{ridge} = \left(\lambda\mathbf{I} + \boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T\mathbf{t}$$

Proof: follow the same approach as for classical regression ■

Ridge Regression: quadratic example



Ridge Regression: quadratic example



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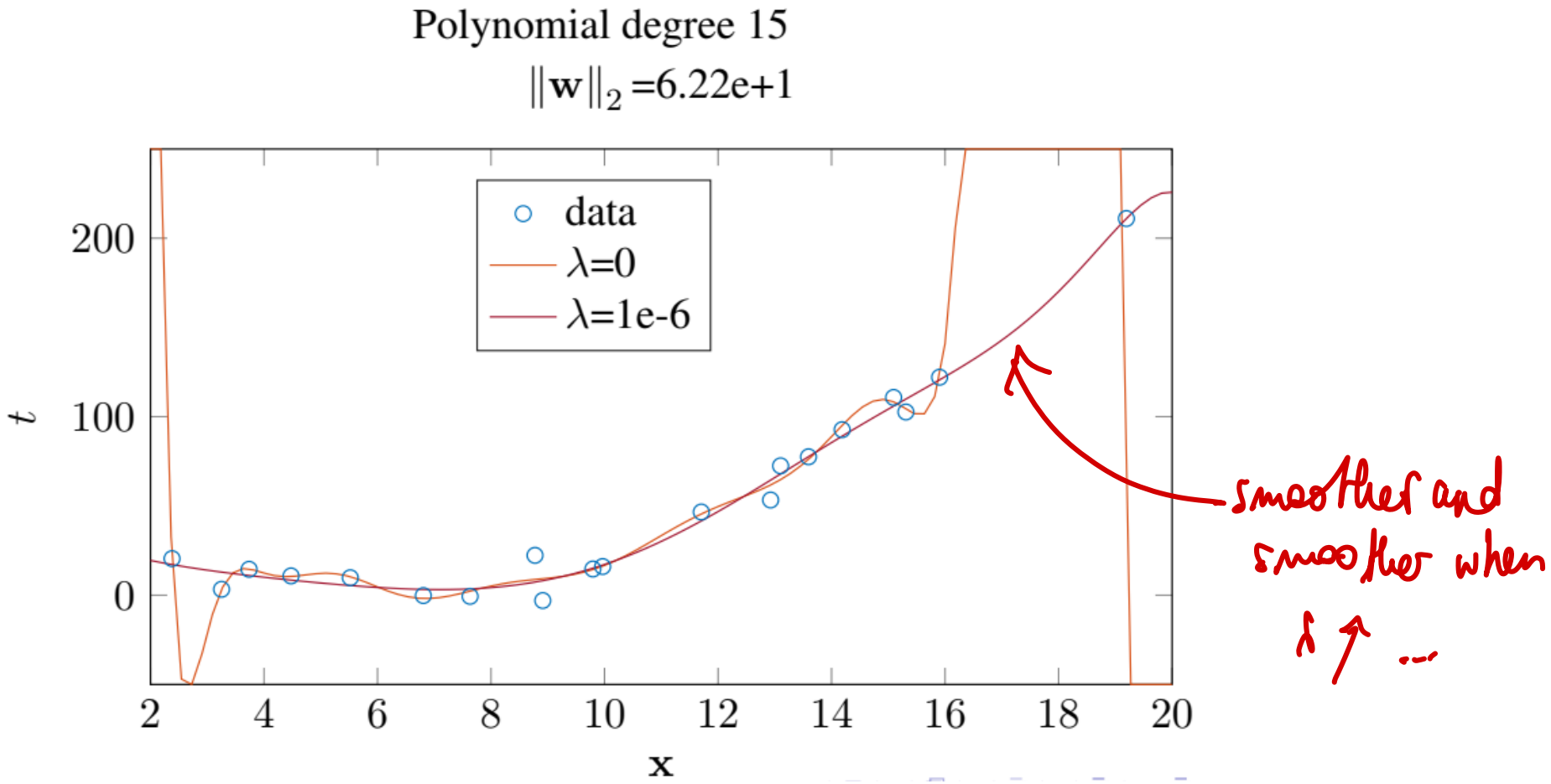

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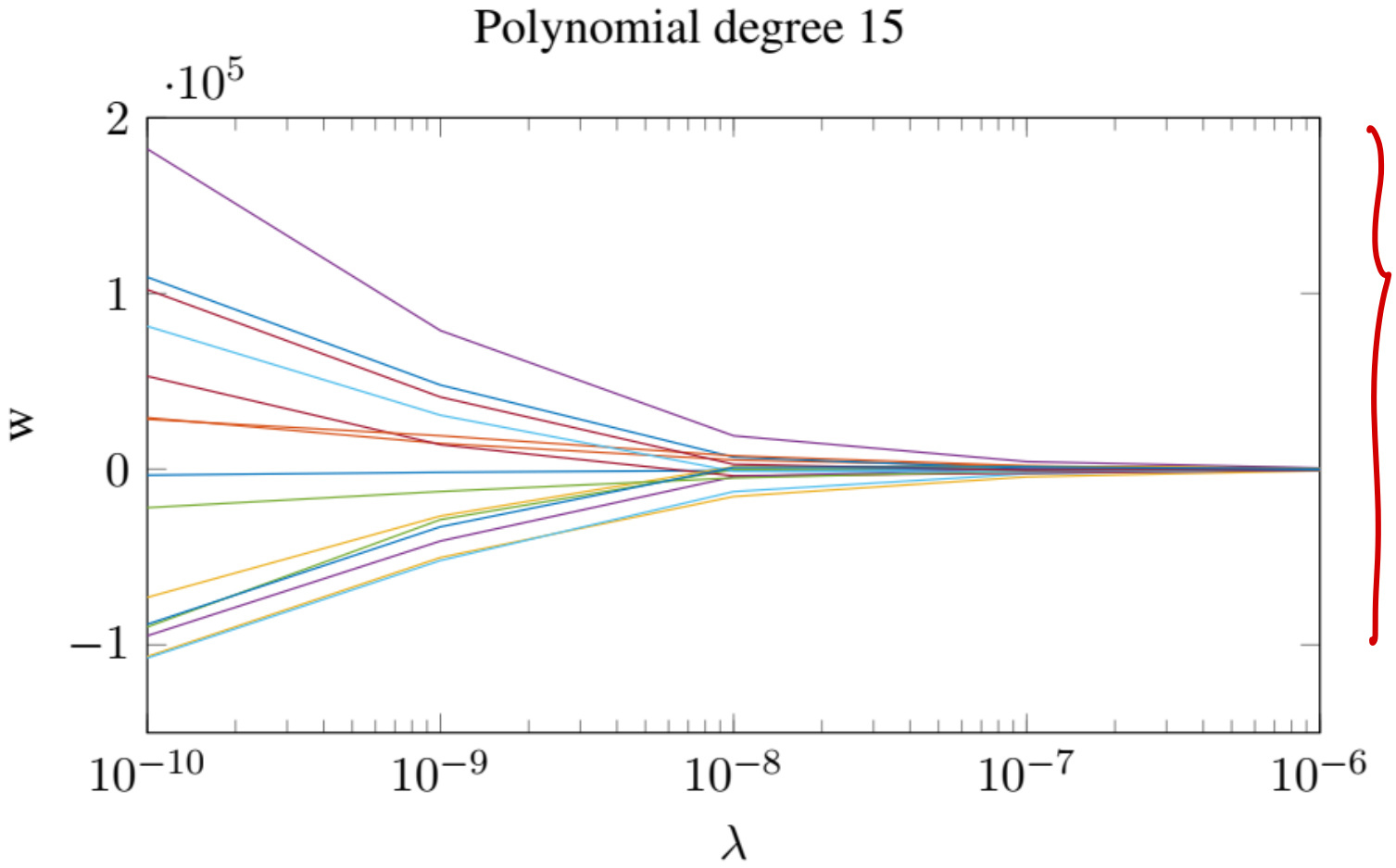


shrinking effects on the weights when ↓ ↑.

2) Lasso → $\|w\|_1$

↳ shrinks almost all weights to 0 ALMOST AT THE SAME SPEED!

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

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

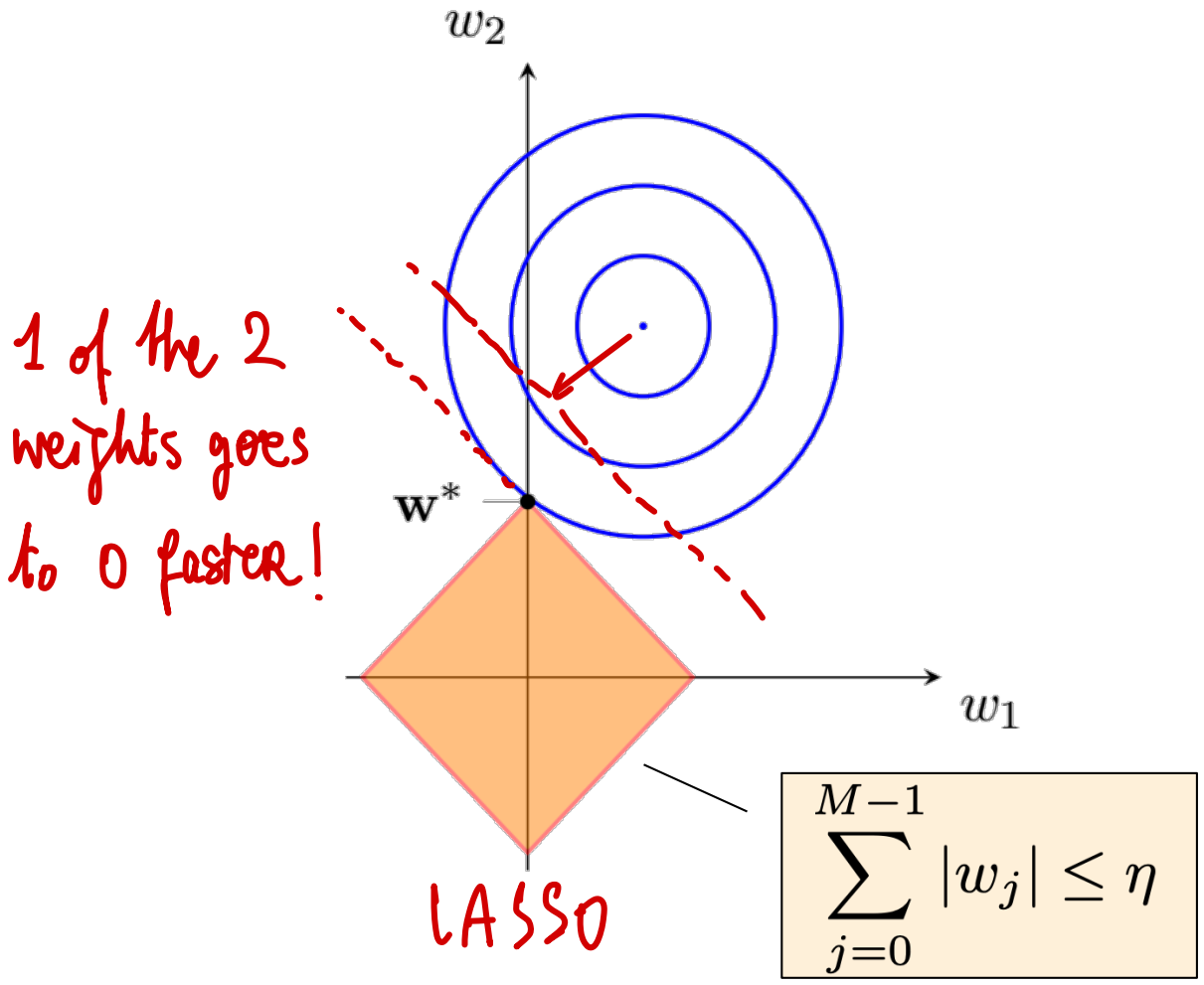
$$\Rightarrow \quad L(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\left(t_i - \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i)\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|_1$$

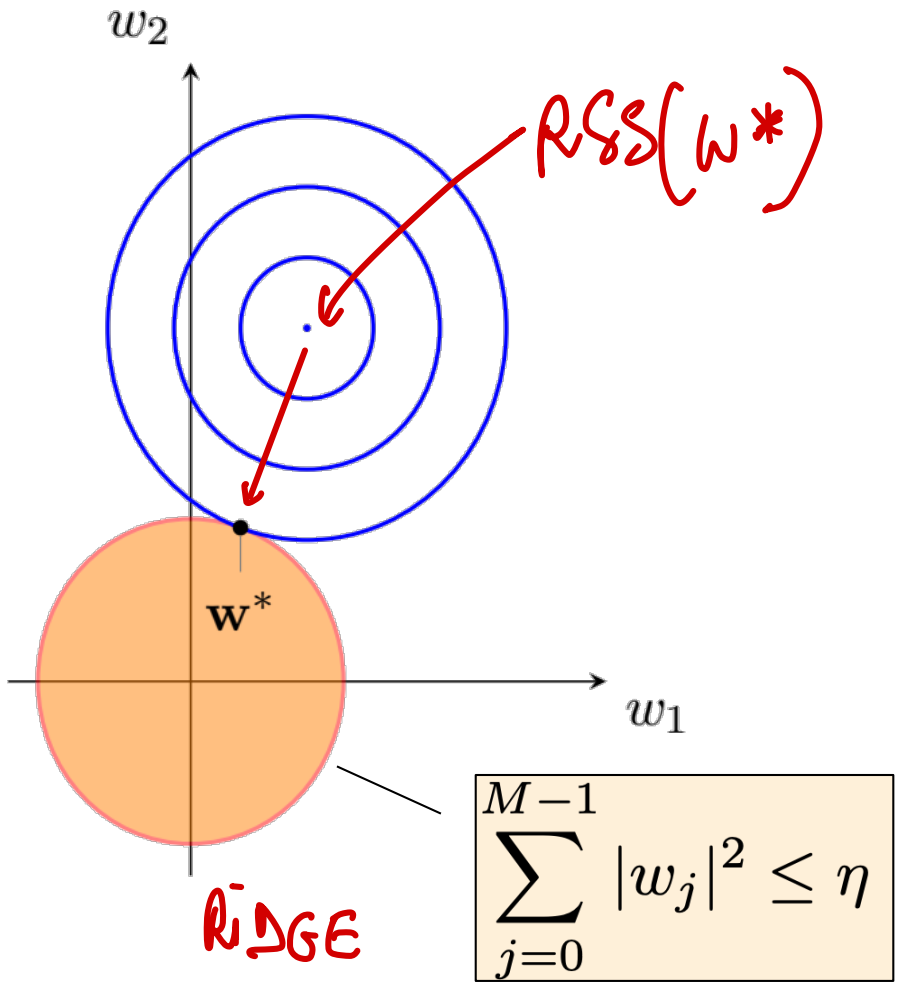
- In this case, closed-form optimization is not possible
- Nevertheless, lasso typically leads to **sparse** regression models: when regularization coefficient (λ) is large enough, some **components** of $\hat{\boldsymbol{w}}$ become **equal to zero**
- We can see regularization equivalent to minimizing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

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

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, $f(x, w)$, 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:

$$\mathbf{w}_{ML} = \arg\max_{\mathbf{w}} p(\mathcal{D}|\mathbf{w})$$

Maximum Likelihood (ML) for linear regression

- Our probabilistic model can be defined as:

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

  - 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 $\mathbf{X}=\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and ouptuts $\mathbf{t}=\{t_1,\ldots,t_N\}^T$:

"μ" of $\mathcal{N}(\mu, \sigma^2)$.

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

By independence

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

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

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

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

no weight dependent

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

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

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

OLS

ML gives birth to the same w* as OLS.

More general probabilistic framework:

Bayesian Linear Regression

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

Parameters Posterior Distribution

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

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

Parameters Posterior Distribution

- 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

on the weights

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

Parameters Posterior Distribution

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

likelihood

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

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

Parameters Posterior Distribution

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

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

in Bayesian Framework I simply look for:

$$w^* = \arg\max_w \left[P(D|w) \right].$$

normalizing constant

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

  - $P(D)$ is the **marginal likelihood** and acts as **normalizing constant**

Parameters Posterior Distribution

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

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

posterior ⇝ what we are trying to model.

  - $p(\mathbf{w}|D)$ 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:

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

Convenient to model the prior via a Gaussian distribution (cf next slide).

Bayesian Linear Regression

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

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

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

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

posterior

"proportional" since we omit the normalising cst.

prior

99% of the time: $w_0 = 0$.

likelihood

Bayesian Linear Regression

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

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$$\Rightarrow \begin{cases} p(\mathbf{w}|\mathbf{t}, \mathbf{\Phi}, \sigma^2) = \mathcal{N}(\mathbf{w}|\mathbf{w}_N, \mathbf{S}_N) & \text{: again a Gaussian.} \\ \mathbf{w}_N = \mathbf{S}_N\left(\mathbf{S}_0^{-1}\mathbf{w}_0 + \dfrac{\mathbf{\Phi}^T\mathbf{t}}{\sigma^2}\right) & \longrightarrow \text{mean.} \\ \mathbf{S}_N^{-1} = \mathbf{S}_0^{-1} + \underbrace{\dfrac{\mathbf{\Phi}^T\mathbf{\Phi}}{\sigma^2}}_{\text{Data}} & \longrightarrow \text{covariance matrix.} \end{cases}$$

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:

cf previously: Maximum Likelihood.

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

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

cf previous slide (expressions)

no assumption at all: ∞ variance for prior.

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

- 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 ($\hat{\mathbf{w}}_{ridge}$) with $\lambda = \frac{\sigma^2}{\tau^2}$

cov. matrix : $S_0 = \begin{bmatrix} \tau^2 & & (0) \\ & \ddots & \\ (0) & & \tau^2 \end{bmatrix}$ → no prior info that leads me to say that there is some kind of correlation.

finite variance.

reg. coeff.

allowing large variance in the weights.

$\tau^2 \nearrow$, $\lambda \searrow$: if you allow large variance you are decreasing the regularization effect.

↳ it's really REGULARIZATION.

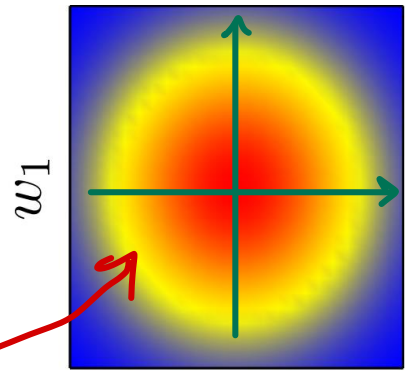
I prefer the ones that have a finite variance, which depends on the value of σ.

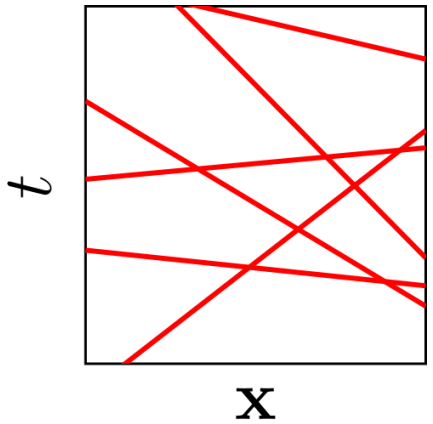
Bayesian Linear Regression: sequential learning

- 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

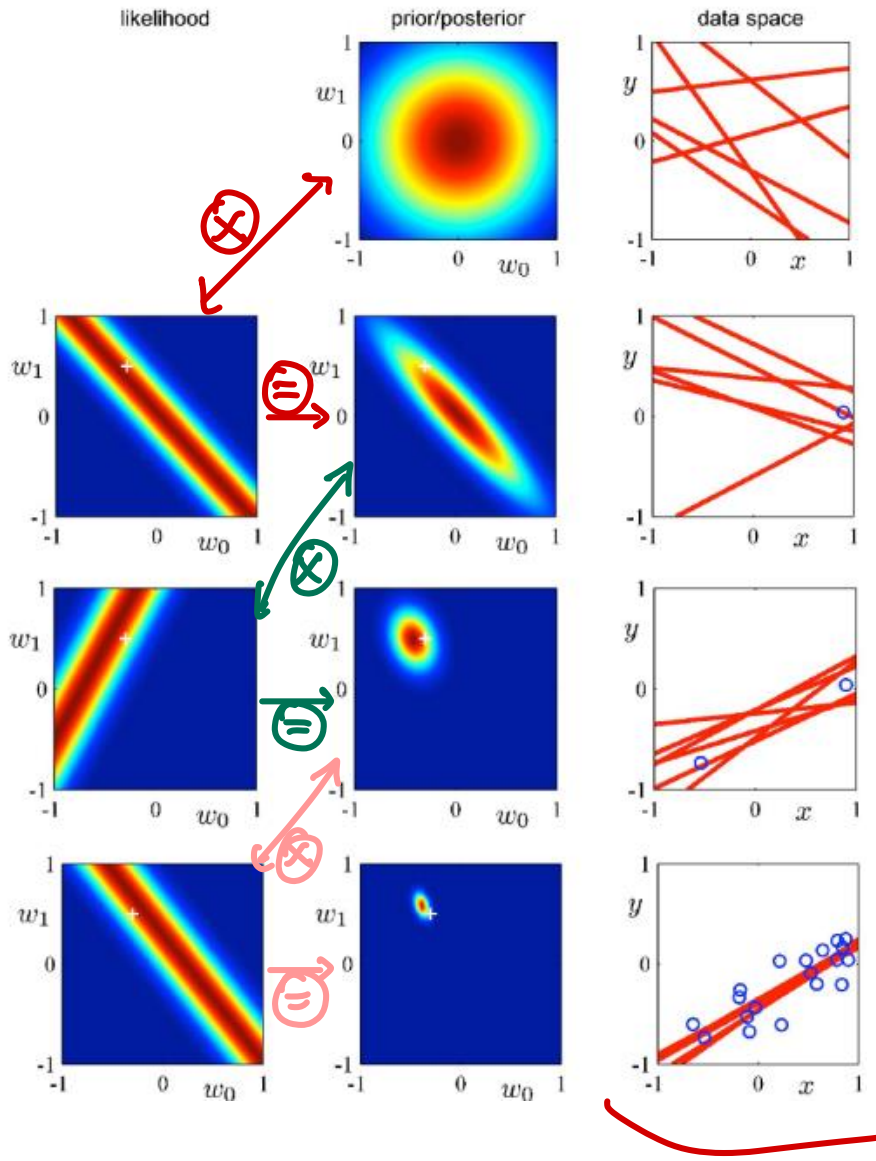
- How to exploit the Bayesian approach for sequential learning?
  - 1) We compute **posterior** with initial data
  - 2) When additional data is available, the **posterior** becomes the **prior**
- Let see an example
  - Let assume data is generated as $t(x) = -0.3 + 0.5x + \varepsilon$
  - Let assume 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 $\mathbf{w_0} = [0,0]^T$





I make solutions close to (0,0) more probable via the prior.

Bayesian Linear Regression: an example (2)



Step 0: 0 samples observed

Step 1: 1 samples observed

Step 2: 2 samples observed

Step 20: 20 samples observed

small variance !

Sequential Learning: the previous posterior becomes the new prior...

I add new data each time ...

Predictive Distribution for Bayesian Regression

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

Tells you that the model is: $t = \mathbf{w}^T \boldsymbol{\phi} + \epsilon$.

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

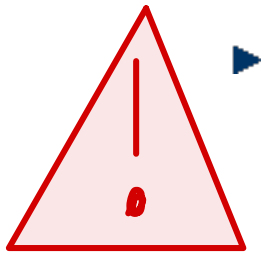
Conditional proba of the target

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

$\mathbf{w}_N{}^T \boldsymbol{\phi}(\mathbf{x})$: E[target] = what my model predicts

$$\Rightarrow \quad \sigma_N^2(\mathbf{x}) = \underbrace{\sigma^2}_{\text{data}} + \underbrace{\boldsymbol{\phi}(\mathbf{x})^T \mathbf{S}_N \boldsymbol{\phi}(\mathbf{x})}_{\text{parameters}}$$ ("uncertainty")

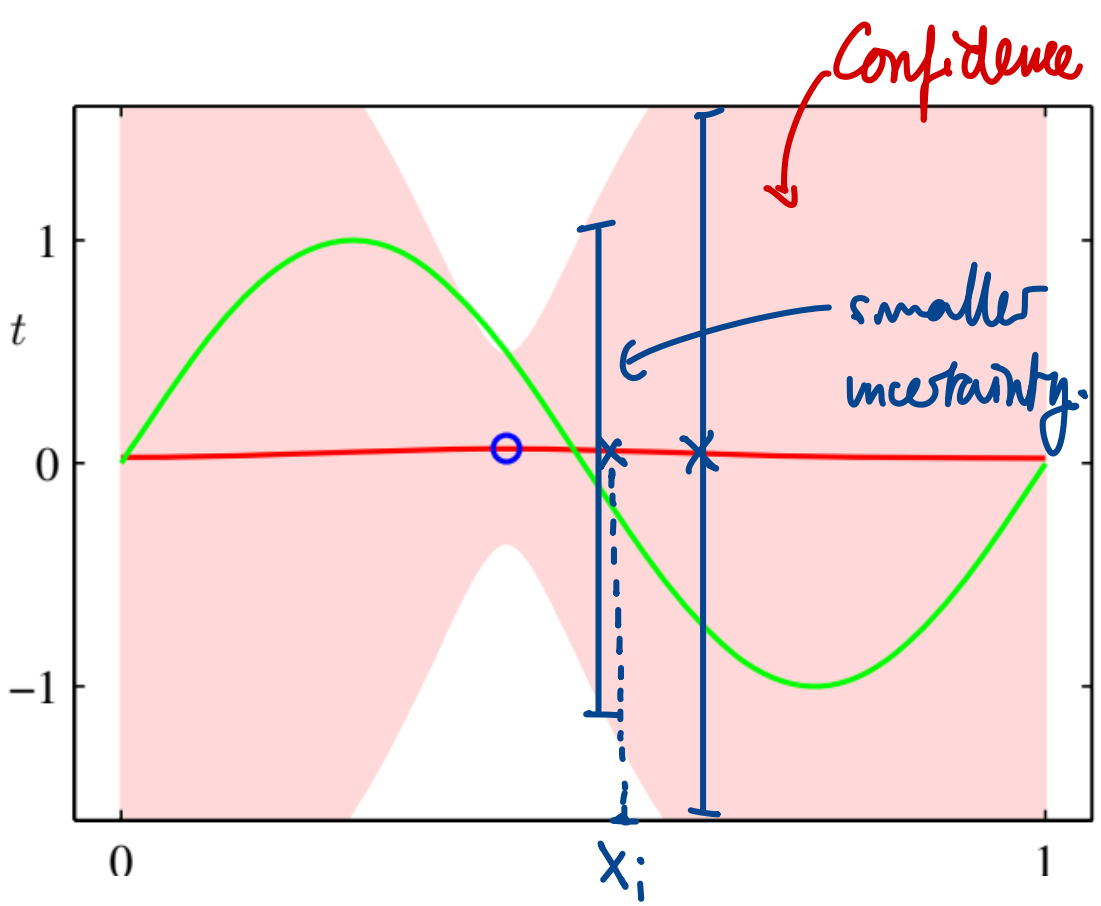
Affected by : data, parameters



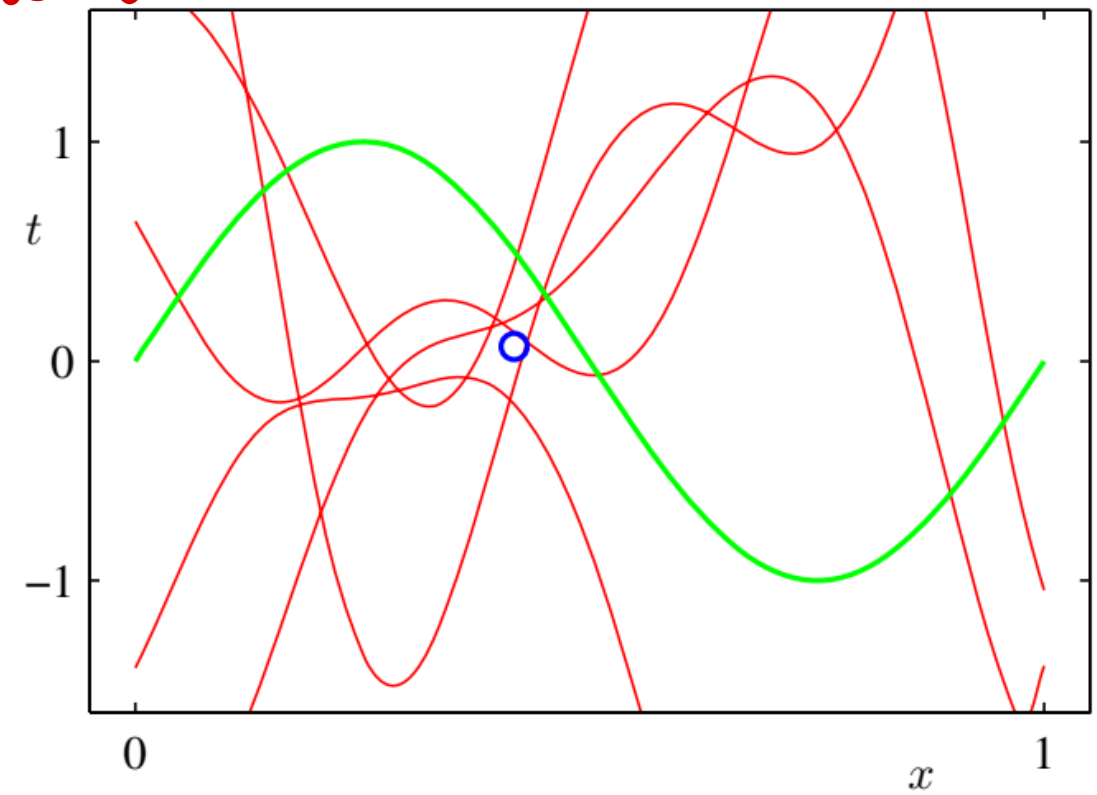
- when $N \to \infty$ the uncertainty associated to parameters (second term) goes to zero and the variance of predictive distribution depends only on variance of data (σ^2)

Predictive Distribution: an example

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



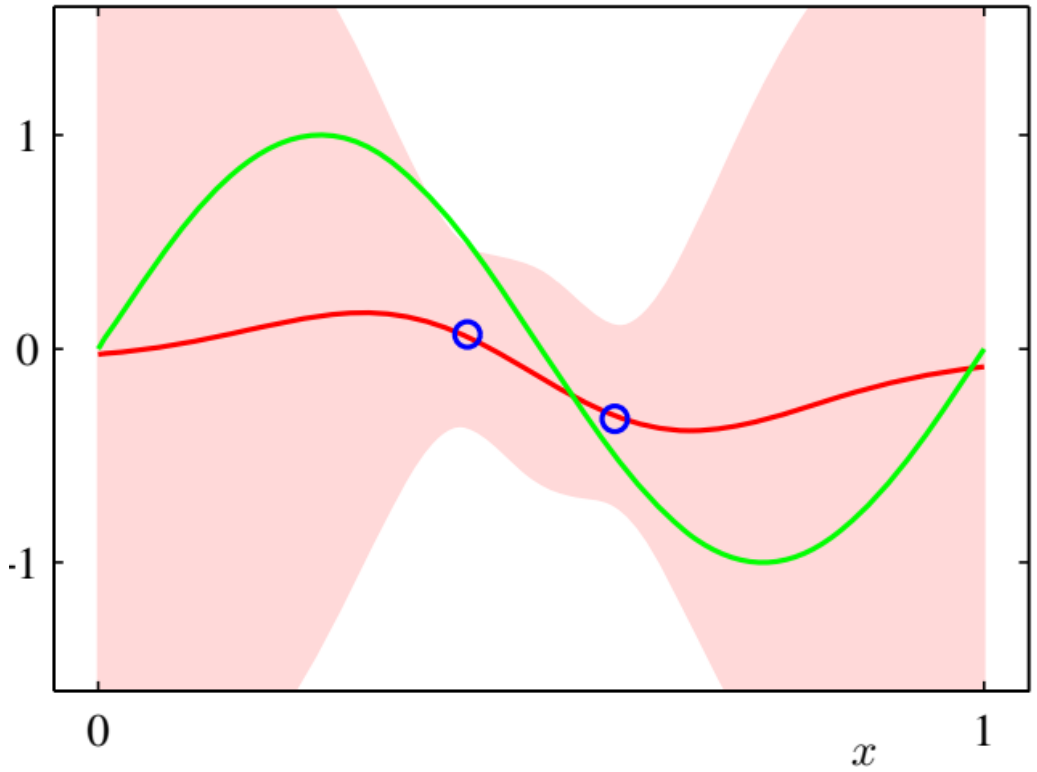
Predictive Distribution



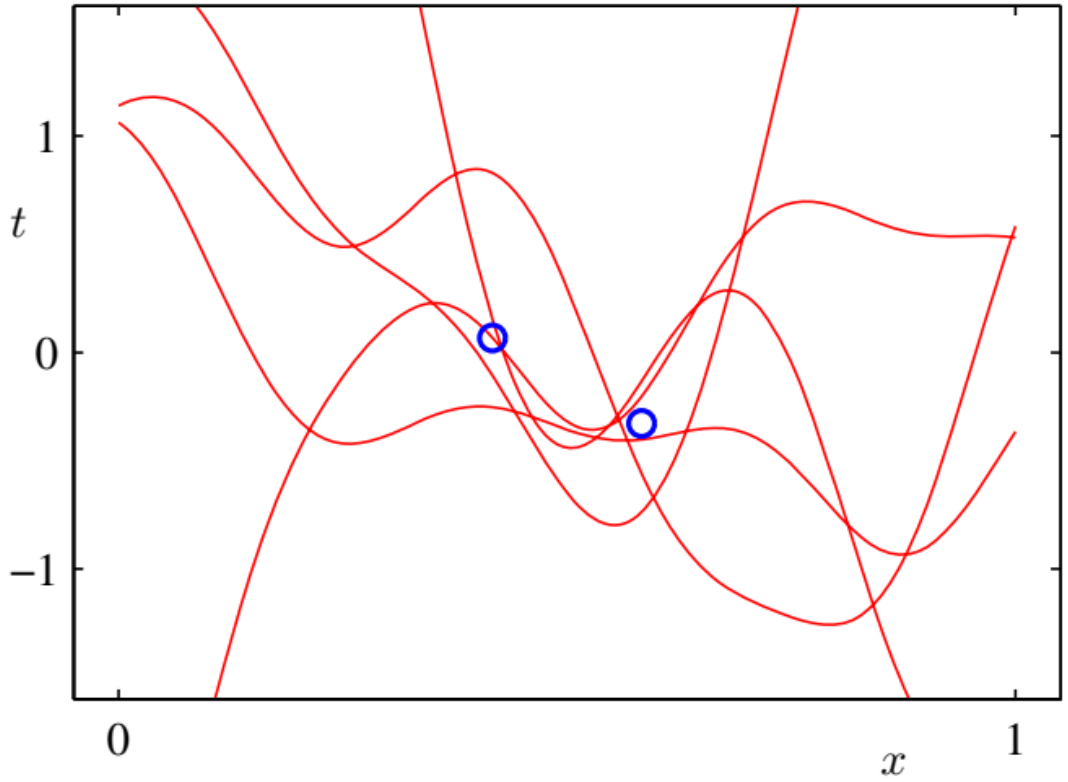
Sampled Models

Predictive Distribution: an example

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



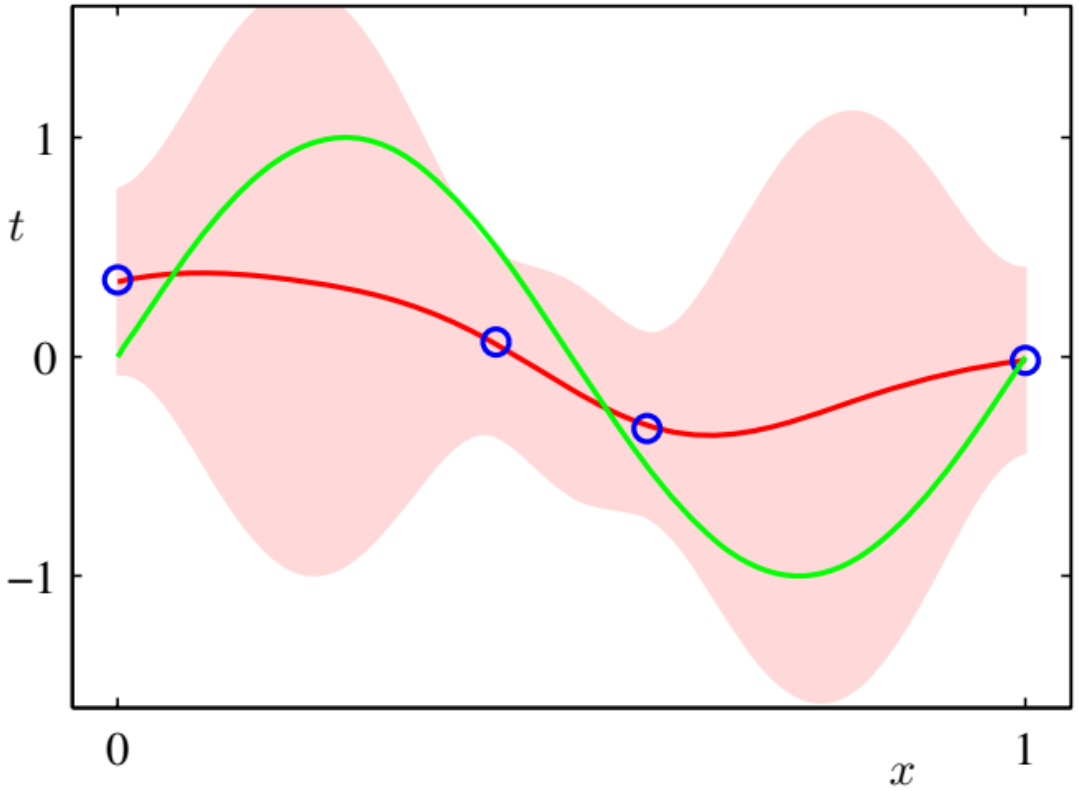
Predictive Distribution



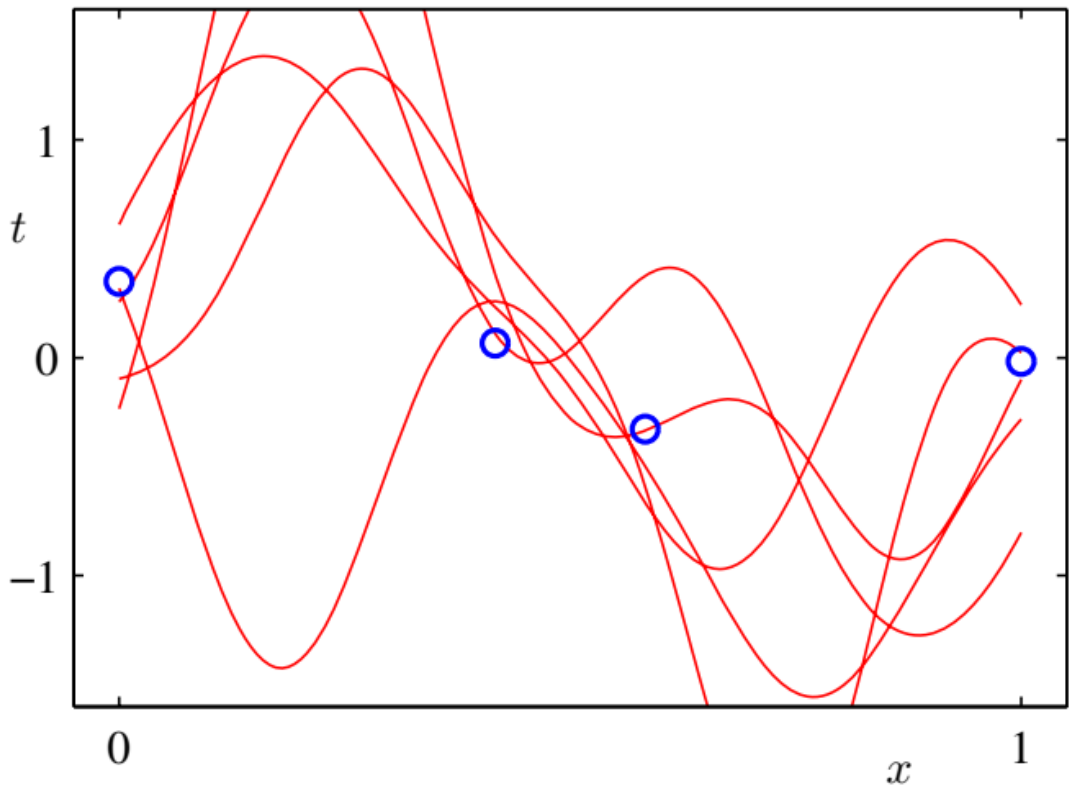
Sampled Models

Predictive Distribution: an example

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



Predictive Distribution

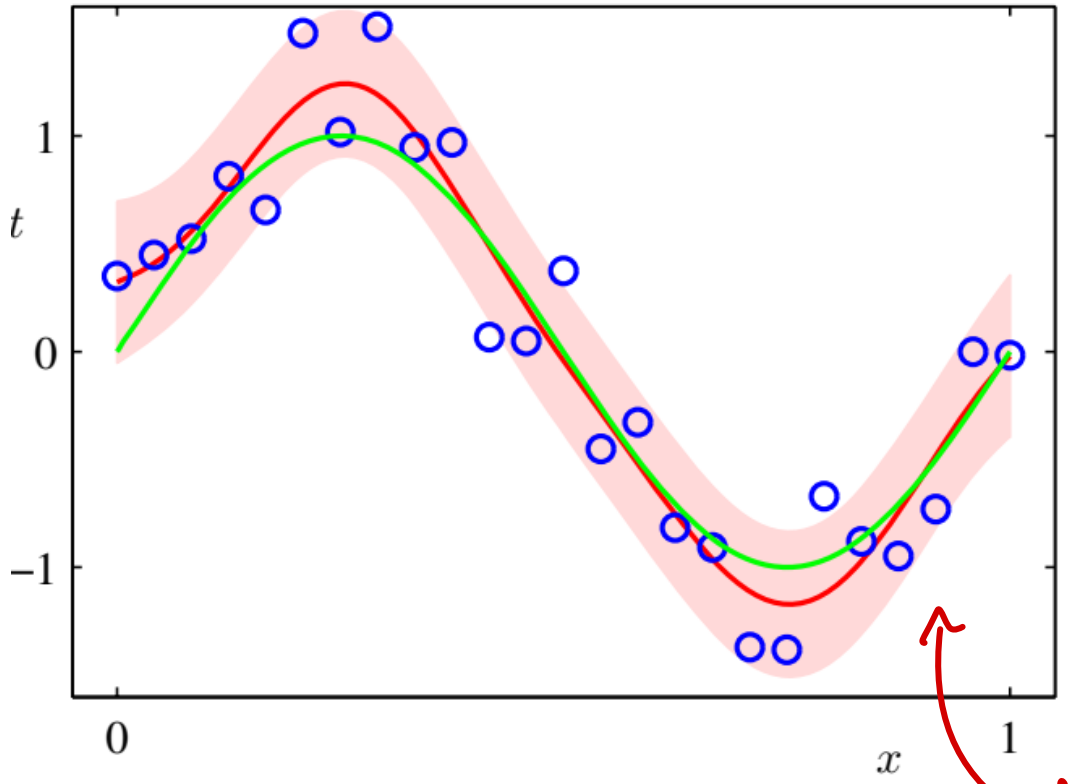


Sampled Models

Predictive Distribution: an example

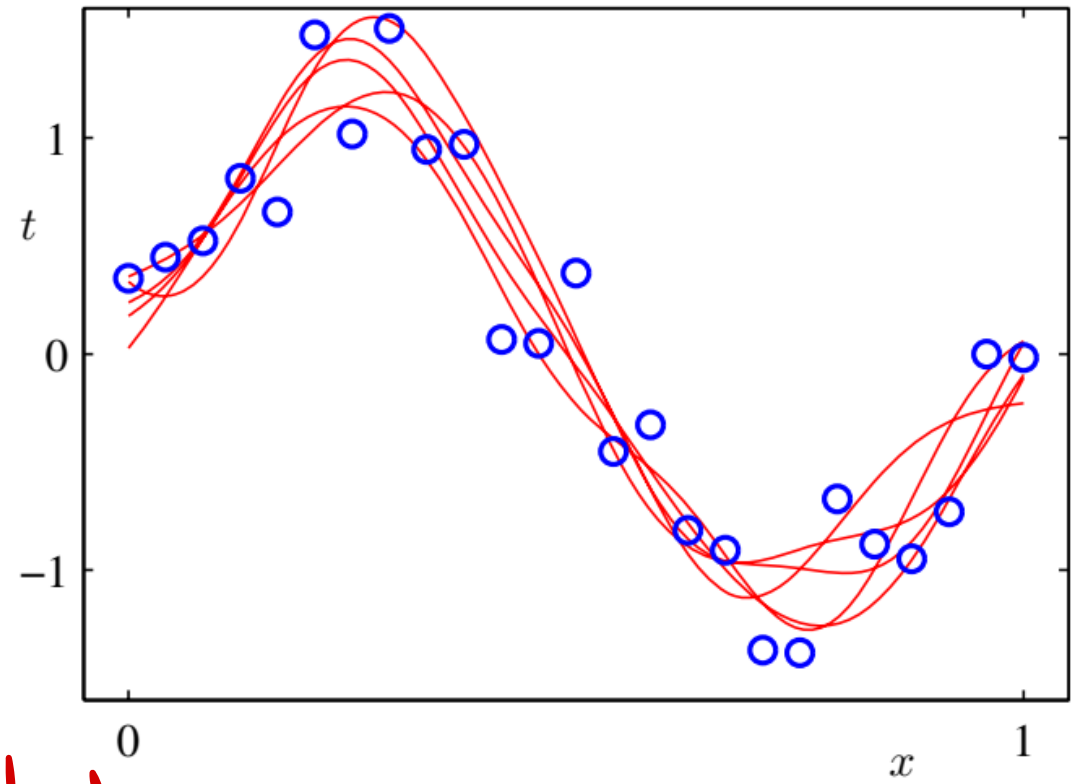
Bayesian framework provides the confidence interval.

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



Predictive Distribution

shrinked confidence interval.



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 integration** 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**