TEXAS A&M UNIVERSITY

CSCE 633: Machine Learning

Lecture 5

Overview

- Linear Regression: Numerical solution
  - General gradient descent
  - Gradient descent for linear regression (batch, stochastic, mini-batch)
- Non-linear basis function for regression

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Linear Regression: Computational Complexity

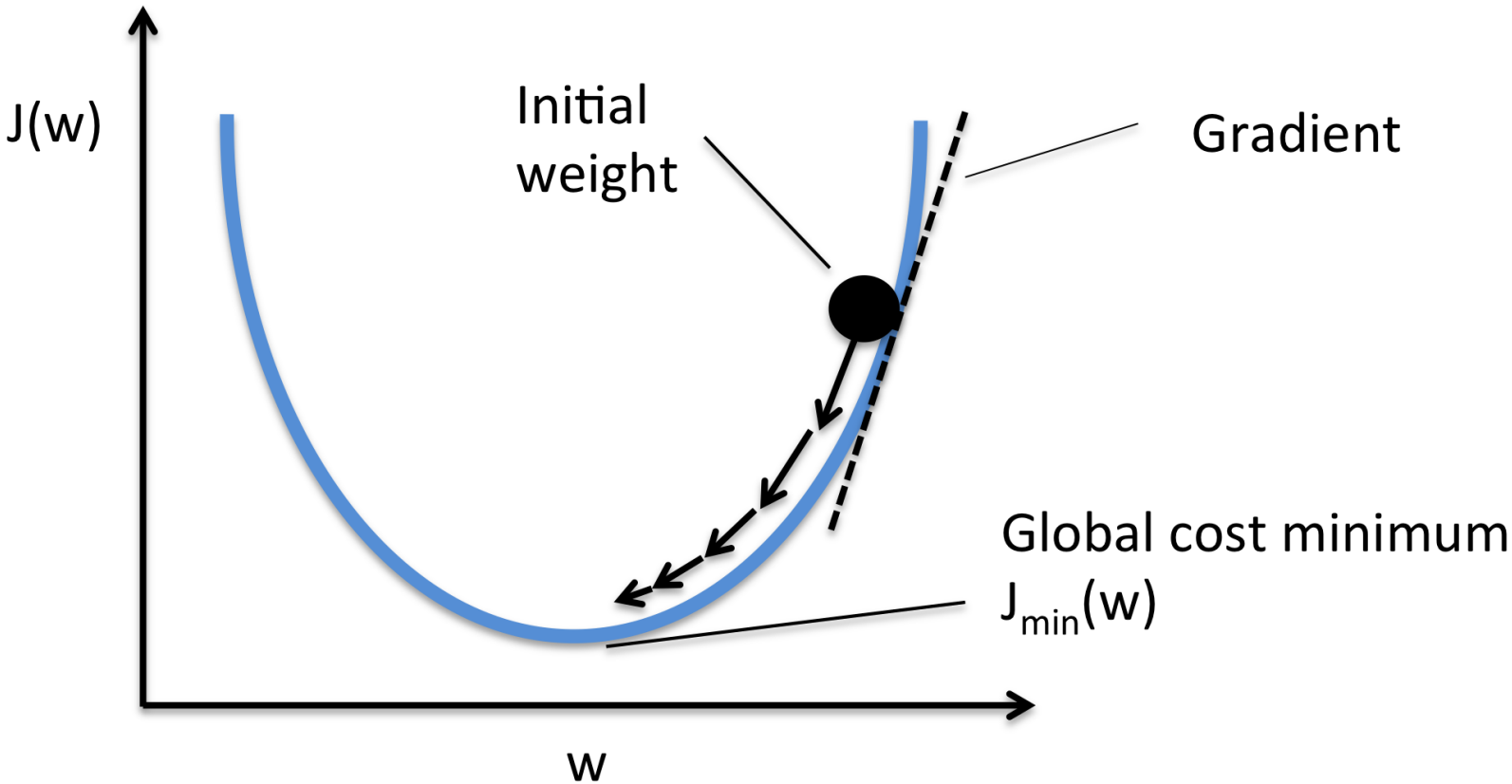
- Bottleneck for computing the solution $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ is to invert the matrix $\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{D\times D}$
- Computational complexity is $O((D+1)^3)$ using Gauss-Jordan elimination
  - Impractical for large D
- Alternative
  - Find approximate solution through an iterative optimization algorithm
  - e.g. Gradient Descent

Gradient Descent

- Iterative algorithm finding a function's minimum via local search
- Standard optimization algorithm in many ML applications
  - e.g. linear regression, logistic regression
  - scales well to large datasets (e.g. no matrix multiplication)
  - proof that it solves many convex problems
  - good heuristic to non-convex problems as well
- **Input:** Function $J(\mathbf{w}) \in \mathbb{R}$
- **Output:** Local minimum $\mathbf{w}^*$
- **Goal:** Minimize $J(\mathbf{w})$ via greedy local search

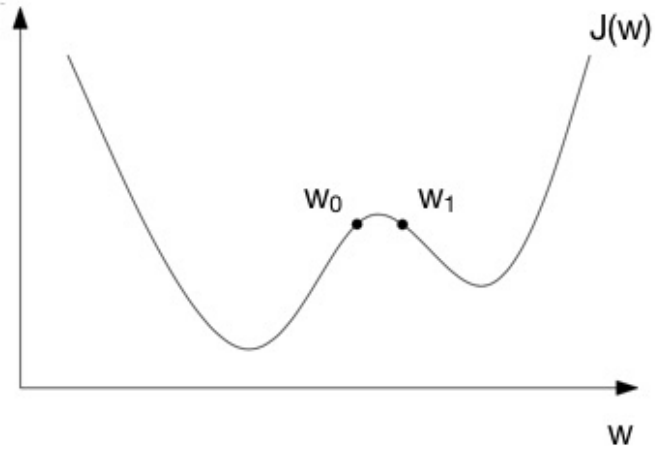
Gradient Descent

1-dimensional example: $J(w) = w^2$



Gradient Descent: 1-dimensional case

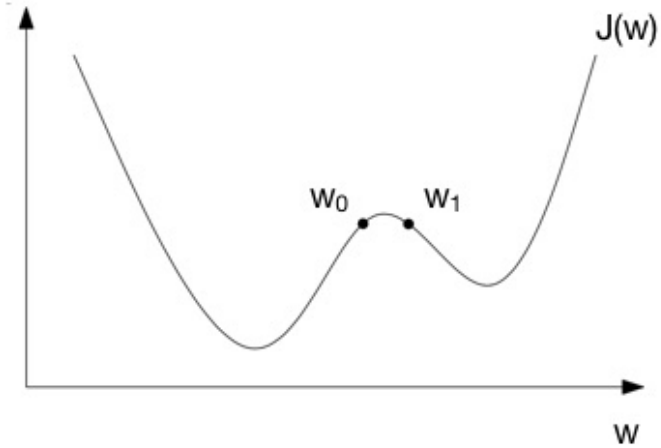
What will happen if we try to minimize $J(w)$ via a local search?



- Starting from w_0
  - We look to the right ($J(w) \uparrow$) and to the left ($J(w) \downarrow$)
  - We take a small step to the left
  - We repeat the above until we reach the left basin
- Starting from w_1
  - We similarly reach the right basin
- It is clear that the outcome depends on the starting point

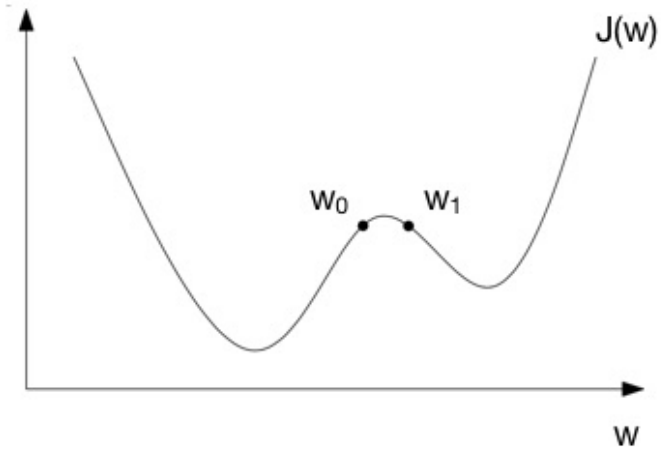
Gradient Descent: 1-dimensional case

More formally, we do the following



- $J'(w) = \frac{dj(w)}{dw} \approx \frac{J(w+\epsilon)-J(w)}{\epsilon}$, for $\epsilon \to 0$ (def. 1^{st} order derivative)
- While $J'(w) \neq 0$
  - If $J'(w) > 0$ (i.e. $J(w+\epsilon) > J(w)$ and $J(w) \uparrow$), move w a little bit to the left
  - If $J'(w) < 0$ (i.e. $J(w+\epsilon) < J(w)$ and $J(w) \downarrow$), move w a little bit to the right
- The derivative $J'(w)$ is used to decide which direction to move
- In other words, move w towards the direction of $-J'(w)$

Gradient Descent: Algorithm Outline



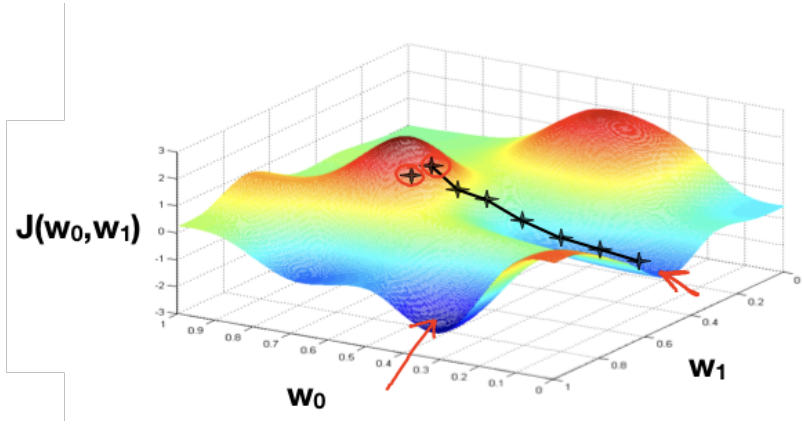
1-dimensional

1 Initialize w, ϵ, $\alpha(\cdot)$, $k := 0$

2 While $|\frac{dJ(w)}{dw}| > \epsilon$

2a $k := k + 1$

2b $w := w - \alpha(k) \cdot \frac{dJ(w)}{dw}$



[Source: Machine Learning, Coursera, Andrew Ng]

d-dimensional

1 Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$

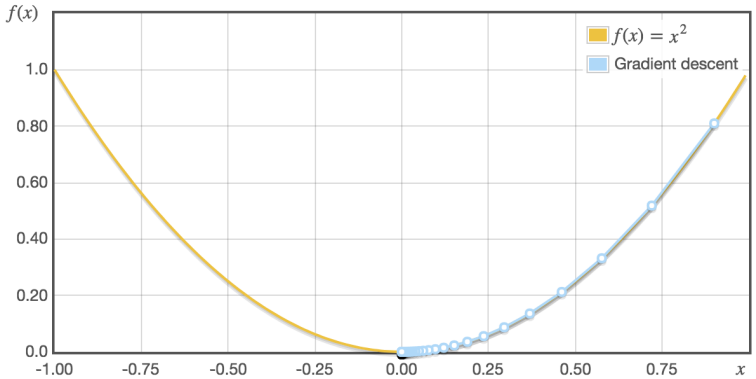
2 While $\|\nabla J(\mathbf{w})\|_2 > \epsilon$

2a $k := k + 1$

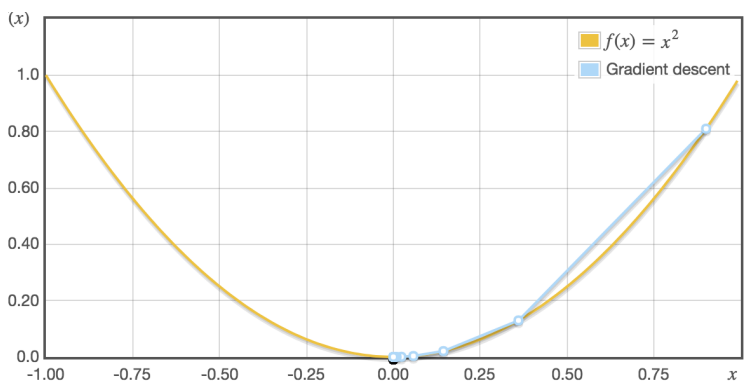
2b $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \nabla J(\mathbf{w})$

Gradient Descent: Step size (or learning rate) α

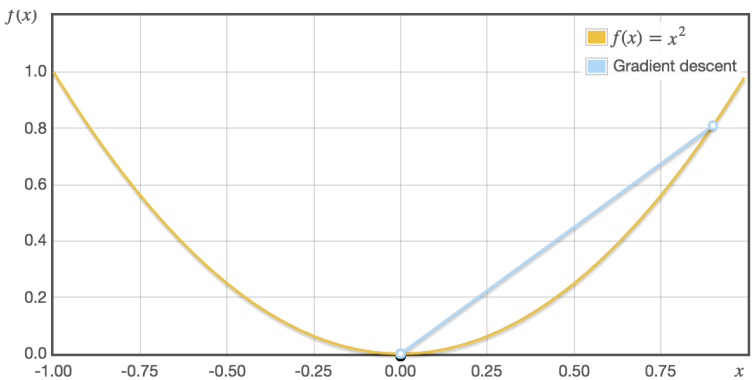
$\alpha = 0.1$



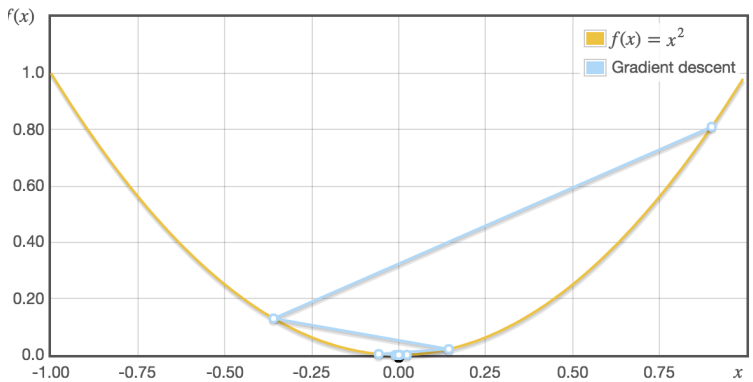
$\alpha = 0.3$



$\alpha = 0.5$



$\alpha = 0.7$



- If $\alpha(k)$ too small, convergence is unnecessarily slow
- If $\alpha(k)$ too large, correction process will overshoot and can diverge

Source: `http://www.onmyphd.com/?p=gradient.descent`

Gradient Descent: Step size (or learning rate) α

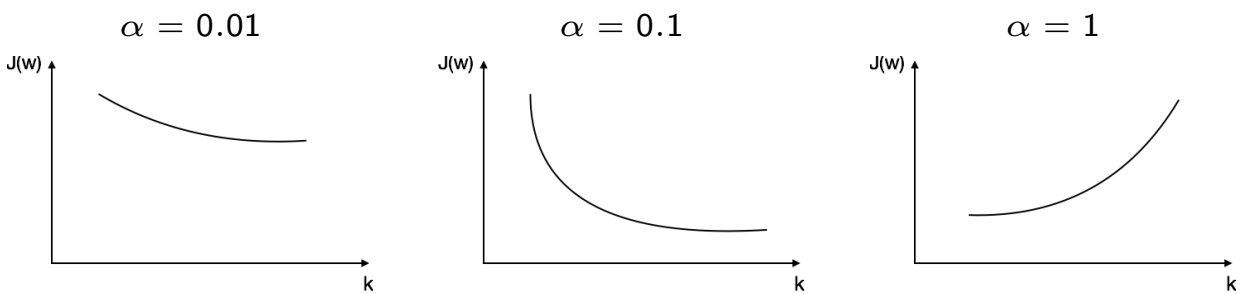
How to chose α?

- In practice, through experimentation
  - Check how $J(\mathbf{w})$ behaves over iterations for multiple α
  - α is a hyper-parameter
  - Therefore it can be tuned using a dev-set or a cross-validation framework

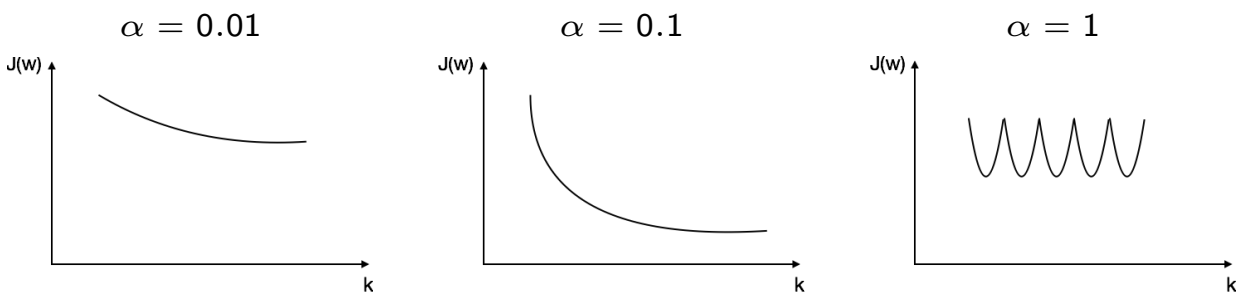
Gradient Descent: Step size (or learning rate) α

Question: A cost function $J(\mathbf{w})$ is optimized with Gradient Descent (GD) using different step size values α. We plot $J(\mathbf{w})$ w.r.t. the number of GD iterations k. Which of the following graph triplets can hold?

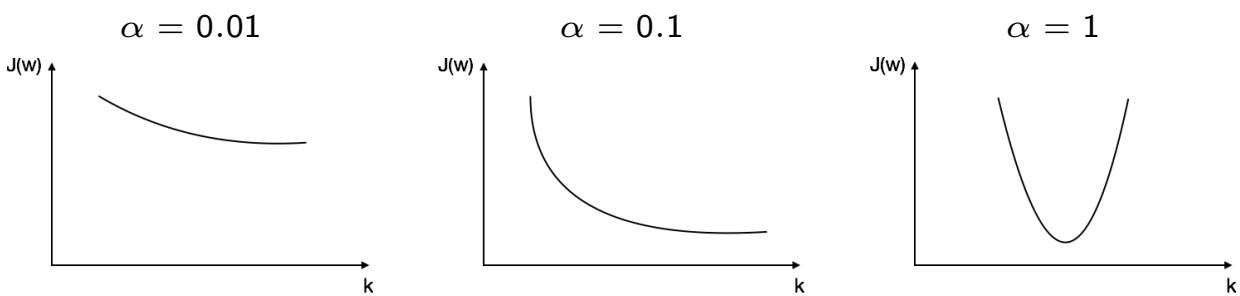
A



B



C



Gradient Descent: Stopping rule

- Hyper-parameter ϵ (i.e. $\|\nabla J(\mathbf{w})\|_2 > \epsilon$) determines when to stop
- Small ϵ: many iterations but higher quality solution
- Large ϵ: less iterations with the cost of more approximate solution
- How to chose ϵ in practice?
  - Try various values to achieve balance between cost and precision
  - Again use some type of cross-validation framework

- Hyperparameters: Parameters set before the beginning of the learning process (e.g. α, ϵ in gradient descent)
- Hyperparameter tuning: The process of choosing a set of optimal hyperparameters for the learning process
- Model parameters: The parameters learned during the learning process (e.g. weights $\mathbf{w}$ in linear regression)

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Gradient Descent in Linear Regression

We can now derive the algorithm outline for minimizing the residual square sum (RSS) error of linear regression with gradient descent

- The residual sum of squares is the cost function:
$$J(\mathbf{w}) = RSS(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$
$$= \mathbf{y}^T\mathbf{y} - 2(\mathbf{X}\mathbf{w})^T\mathbf{y} + (\mathbf{X}\mathbf{w})^T(\mathbf{X}\mathbf{w})$$
$$= \mathbf{y}^T\mathbf{y} - 2\mathbf{w}^T(\mathbf{X}^T\mathbf{y}) + \mathbf{w}^T(\mathbf{X}^T\mathbf{X})\mathbf{w}$$
- Gradient Descent optimization expression:
$$\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \nabla J(\mathbf{w})$$
$$\nabla J(\mathbf{w}) = \frac{\vartheta RSS(\mathbf{w})}{\vartheta \mathbf{w}} = -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\mathbf{w}$$

Gradient Descent in Linear Regression

Question: Derive the algorithm outline for minimizing the residual square sum (RSS) error of linear regression with gradient descent

(Batch) Gradient Descent for Linear Regression

1 Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$

2 While $\|\nabla RSS(\mathbf{w})\|_2 > \epsilon$

2a $k := k + 1$

2b $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot (\mathbf{X}^T\mathbf{X}\mathbf{w} - \mathbf{X}^T\mathbf{y})$

Gradient Descent in Linear Regression

Stochastic Gradient Descent for Linear Regression

Update weights using one sample at a time

1. Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$
2. Loop until convergence
   - 2a $k := k + 1$
   - 2b Randomly choose a sample $(\mathbf{x_i}, y_i)$
   - 2c Compute its contribution to the gradient $\mathbf{g_i} = (\mathbf{x_i}^T \mathbf{w} - y_i) \cdot \mathbf{x_i}$
   - 2d Update the weights $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \mathbf{g_i}$

Gradient Descent in Linear Regression

Mini-Batch Gradient Descent for Linear Regression

Update weights using subset of samples at a time

1. Initialize $\mathbf{w}$, ϵ, $\alpha(\cdot)$, $k := 0$
2. Loop until convergence
   - 2a $k := k + 1$
   - 2b Randomly choose a subset of samples $S = \{(\mathbf{x_i}, y_i), \ldots, (\mathbf{x_{i+M}}, y_{i+M})\}$
   - 2c Form the mini-batch data matrix $\mathbf{X_S} = \begin{bmatrix} \mathbf{x_i}^T \\ \vdots \\ \mathbf{x_{i+M}}^T \end{bmatrix}$
   - 2d Update the weights $\mathbf{w} := \mathbf{w} - \alpha(k) \cdot \left(\mathbf{X_S}^T \mathbf{X_S} \mathbf{w} - \mathbf{X_S}^T \mathbf{y} \right)$

- Good compromise between batch and stochastic gradient descent
- Common mini-batch sizes range between M=50-250 samples

Gradient Descent in Linear Regression

- Batch gradient descent computes exact gradient
- Stochastic gradient descent
  - Computes approximate gradient using one sample per iteration
  - Its expectation equals the true gradient
- Mini-batch gradient descent
  - Computes gradient based on subset of samples
- For large-scale problems stochastic or mini-batch descent often work well

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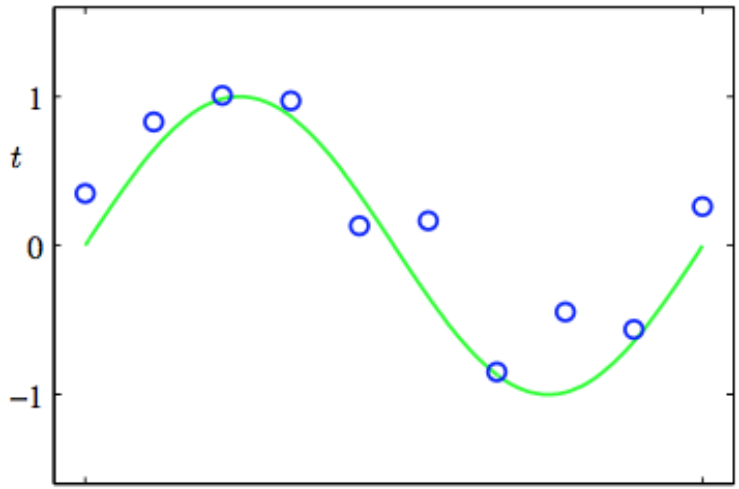
What if data does not fit a line?

Example: Samples from a sine function



We can use a non-linear basis function

$\phi(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^D \rightarrow \mathbf{z} \in \mathbb{R}^M$

We can apply our linear regression model to the new features

$y_i = \mathbf{w}^T \mathbf{z_i} = \mathbf{w}^T \phi(\mathbf{x_i})$

$RSS(\mathbf{w}) = \sum_{n=1}^{N} \left(y_i - \mathbf{w}^T \phi(\mathbf{x_i})\right)^2, \ \mathbf{w} \in \mathbb{R}^M$

Example: $\mathbf{x} = [x_1, x_2]^T \in \mathbb{R}^2, \ \phi(\mathbf{x}) = [x_1, x_2^2, x_1^3 + x_2]^T \in \mathbb{R}^3$

Non-Linear Basis Function

Residual sum of squares

$$RSS(\mathbf{w}) = \sum_{n=1}^{N} \left(y_i - \mathbf{w}^T \phi(\mathbf{x_i})\right)^2 = (\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})^T(\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})$$

Non-linear design matrix

$$\boldsymbol{\Phi} = \begin{bmatrix} \phi(\mathbf{x_1})^T \\ \phi(\mathbf{x_2})^T \\ \vdots \\ \phi(\mathbf{x_N})^T \end{bmatrix} \in \mathbb{R}^{N \times M}$$

LMS solution with the non-linear design matrix

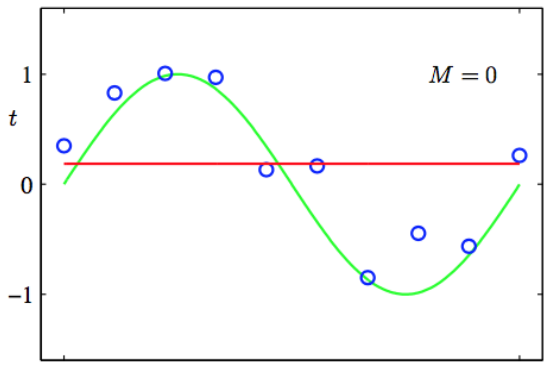
$$\mathbf{w}^{LMS} = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{y}$$

Non-Linear Basis Function

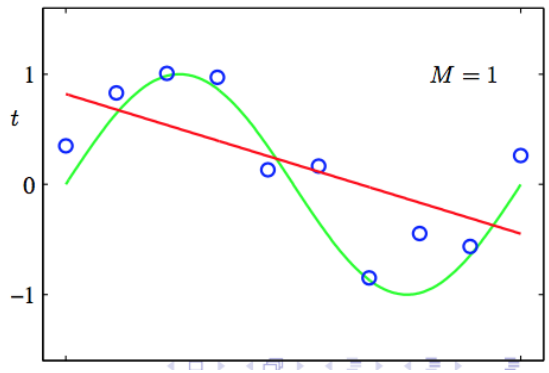
Example: Samples from a sine function

Polynomial basis function $\phi(\mathbf{x}) = [1\ x\ \ldots\ x^M]^T$

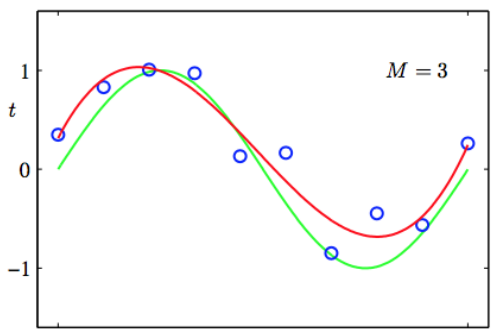
$M = 0$ underfitting



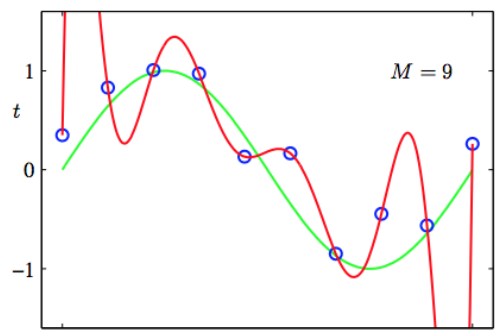
$M = 1$ underfitting



$M = 3$



$M = 9$ overfitting



Overfitting

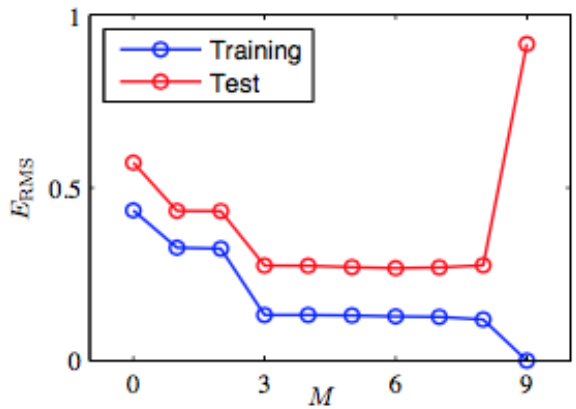
Weights of high order polynomials are very large

$$y_i = \mathbf{w}^T \mathbf{z_i} = \mathbf{w}^T \phi(\mathbf{x_i}), \quad \mathbf{z_i} = \phi(\mathbf{x_i}) \in \mathbb{R}^M$$

	$M=0$	$M=1$	$M=3$	$M=9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
w_5				640042.26
w_6				-1061800.52
w_7				1042400.18
w_8				-557682.99
w_9				125201.43

Overfitting

- The risk of using highly flexible (complicated) models without enough data
- Leads to poor generalization
- How to detect overfitting?
  - Plot model complexity (e.g. polynomial order) versus objective function
  - As complexity increases, performance on training improves, while on testing first improves and then deteriorates
- How to avoid overfitting?
  - More data or regularization

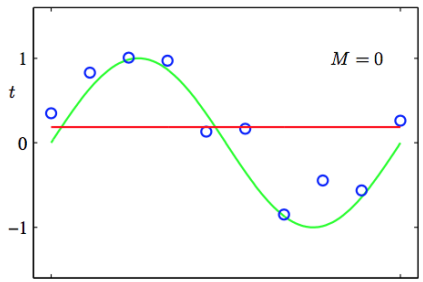


Overfitting

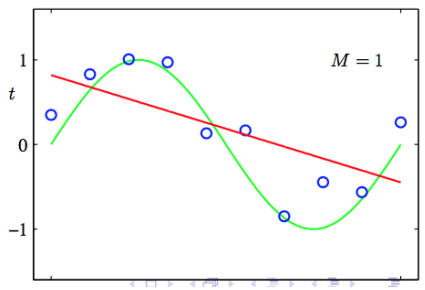
Example: Non-linear regression $y = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M$

Samples from a sine function $x_i = \sin(t_i)$, $t_i \sim \text{Uniform}(0, 2\pi)$

$M = 0$ underfitting



$M = 1$ underfitting



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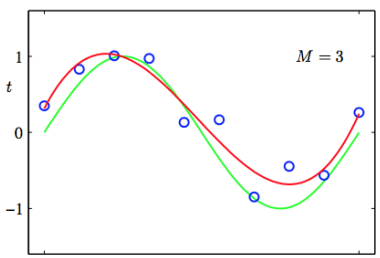
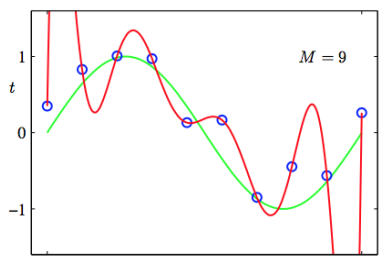
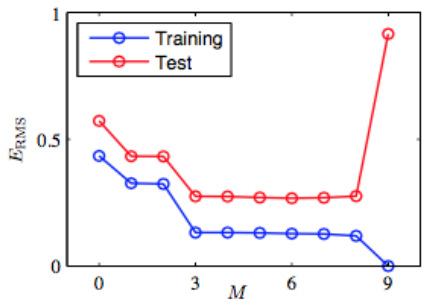
$M = 3$



$M = 9$ overfitting



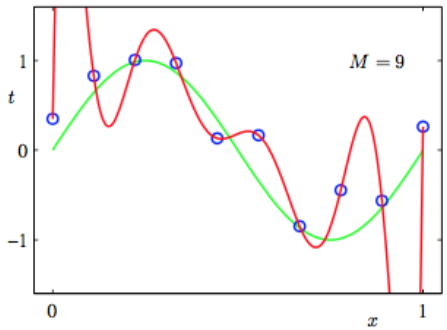


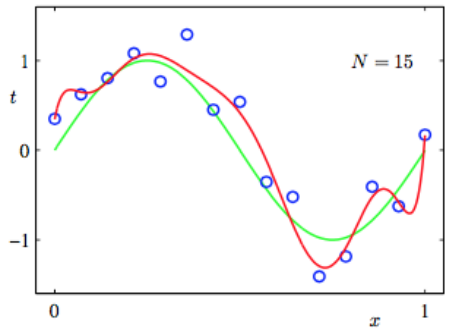
As model becomes more complex, performance on training keeps improving while on test data improve first and deteriorate later.

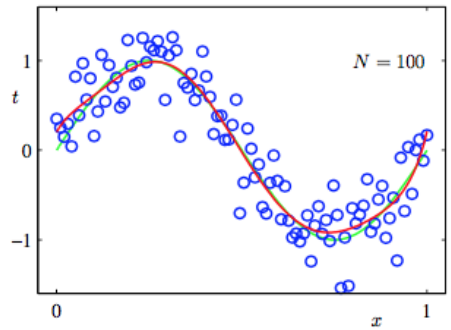
The larger a coefficient w_i, the easier for the model to "swing" in that dimension, increasing chance to fit more noise.

How can we avoid overfitting?

One solution: Use more training data







What if we don't have a lot of data?

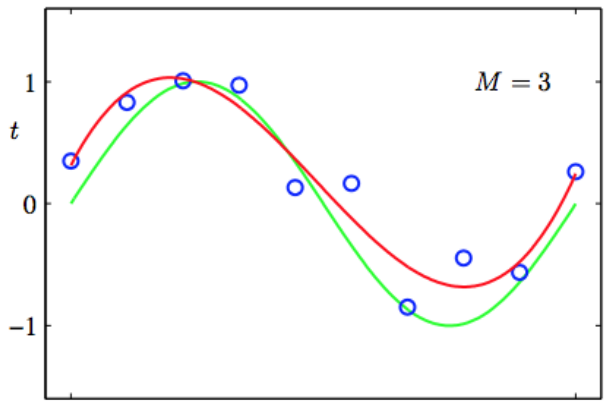
Another solution: Use less features (e.g. feature selection algorithms)

Intuitively, this will reduce the complexity of the model, therefore it is likely to result in less overfitting.

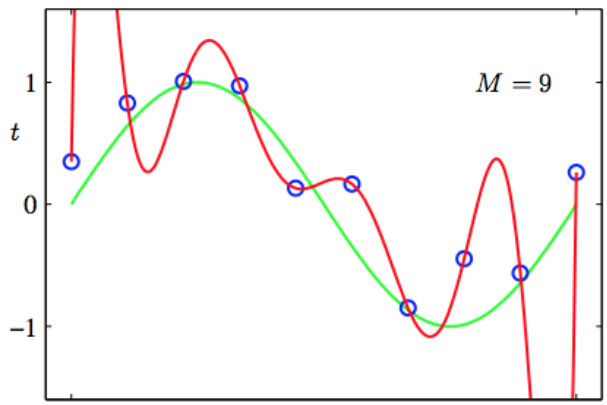
How can we avoid overfitting?

A more general solution: Regularization

$M = 3$



$M = 9$



$y = w_0 + w_1 x + w_2 x^2$ $\quad$ $y = w_0 + w_1 x + w_2 x^2 + \ldots + w_9 x^9$

How about penalizing and making small $w_3, \ldots, w_9$?

The cost function to be minimized would become:

$J(\mathbf{w}) = RSS(\mathbf{w}) + w_3^2 + \ldots w_9^2$

But we may not know in advance which parameters we want to penalize

$\rightarrow$ So we can penalize them all

How can we avoid overfitting?

A more general solution: Regularization

Suppose we have a learning model whose evaluation criterion $EC(\mathbf{w})$ we want to optimize with respect to weights $\mathbf{w} = [w_1, \ldots, w_D]^T$

- $J(\mathbf{w}) = EC(\mathbf{w}) + \lambda \sum_{d=1}^{D} w_d^2 = EC(\mathbf{w}) + \lambda \|\mathbf{w}\|_2^2$
  $\rightarrow$ l2-norm regularization
- $J(\mathbf{w}) = EC(\mathbf{w}) + \frac{\lambda}{N} \sum_{d=1}^{D} w_d^2$
  (as #data N increases, we need to worry less about overfitting)
- $J(\mathbf{w}) = EC(\mathbf{w}) + \lambda \sum_{d=1}^{D} \|w_d\| = EC(\mathbf{w}) + \lambda \|\mathbf{w}\|$
  $\rightarrow$ l1-norm regularization

Evaluation criterion $EC(\mathbf{w})$ can be RSS or log-likelihood for linear regression, negative cross-entropy for logistic regression, etc.

$\lambda \geq 0$ is the model complexity penalty

Regularization for Non-Linear Regression

l2-norm regularization

Linear: $J(\mathbf{w}) = RSS(\mathbf{w}) + \lambda\|\mathbf{w}\|_2^2 = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w}) + \lambda\|\mathbf{w}\|_2^2$

Non-linear: $J(\mathbf{w}) = RSS(\mathbf{w}) + \lambda\|\mathbf{w}\|_2^2 = (\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})^T(\mathbf{y} - \boldsymbol{\Phi}\mathbf{w}) + \lambda\|\mathbf{w}\|_2^2$

Closed-form solution:

Linear: $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}_{D\times D})^{-1}\mathbf{X}^T\mathbf{y}$

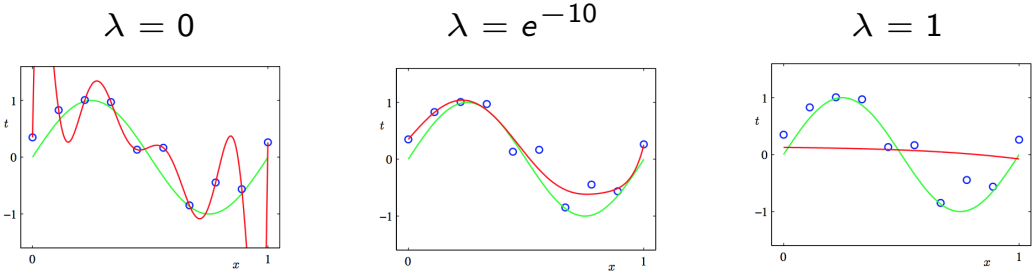
Non-linear: $\mathbf{w}^* = (\boldsymbol{\Phi}^T\boldsymbol{\Phi} + \lambda\mathbf{I}_{D\times D})^{-1}\boldsymbol{\Phi}^T\mathbf{y}$

The above reduces to ordinary least squares (OLS) solution when $\lambda = 0$ (see handout for derivation)

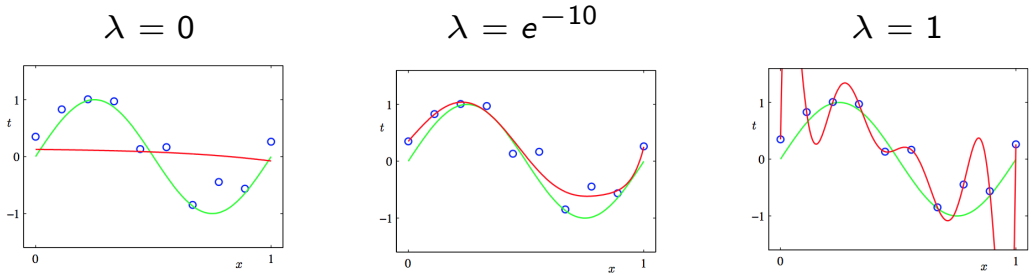
Regularization for Non-Linear Regression

Question: Assume a set of samples generated from a sine function $x_i = \sin(t_i)$ (green line), modeled with **regularized** non-linear regression $y = w_0 + w_1 x + \ldots + w_9 x^9$. How does the resulting model (red line) look as we increase the amount of regularization λ?

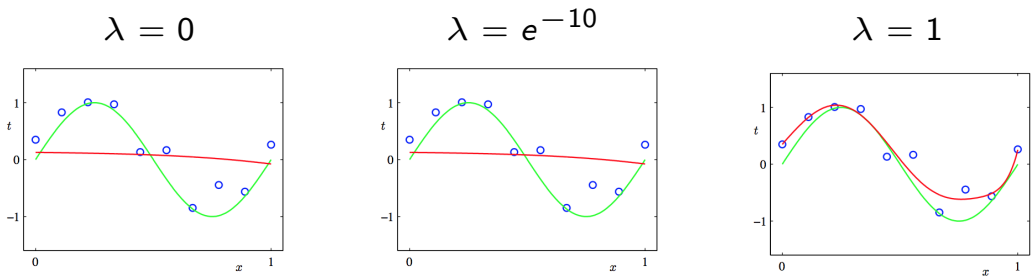
A)



B)



C)



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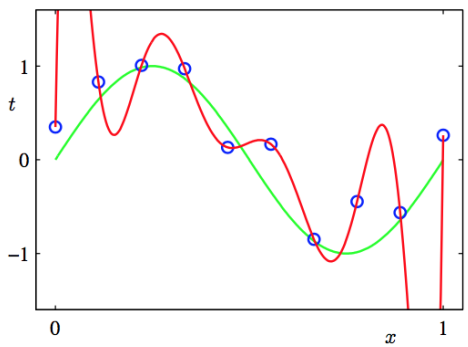
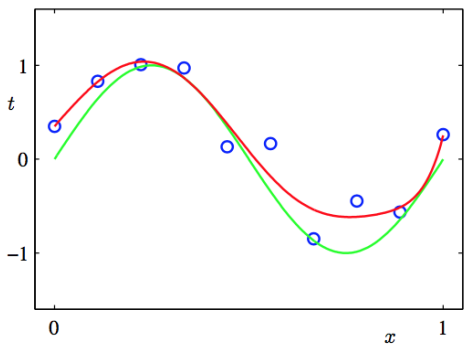
The correct answer is A

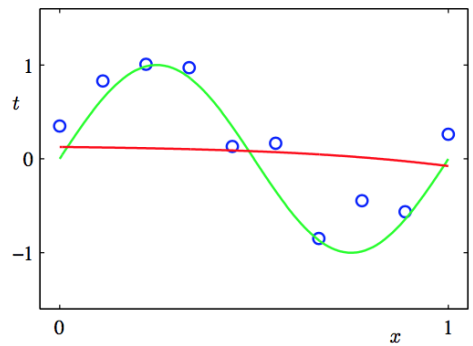
$\lambda = 0$: no regularization



$\lambda = e^{-18}$



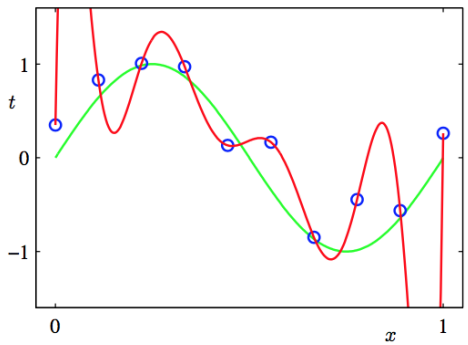
$\lambda = 1$: underfitting



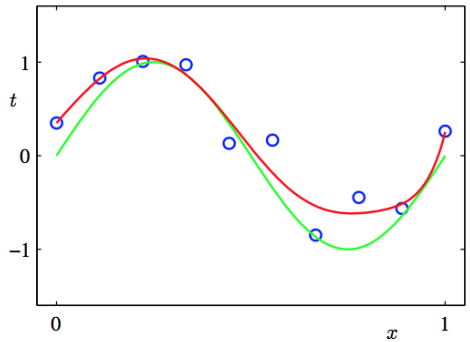
Overfitting is reduced with the help of increasing regularizers

Regularization for Non-Linear Regression

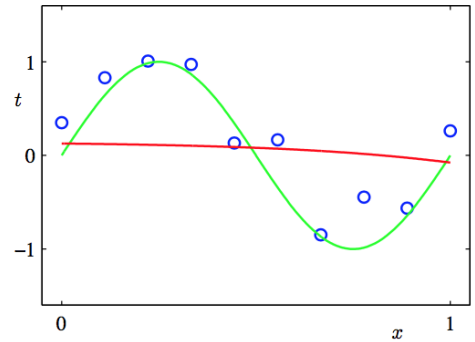
$\lambda = 0$: no regularization

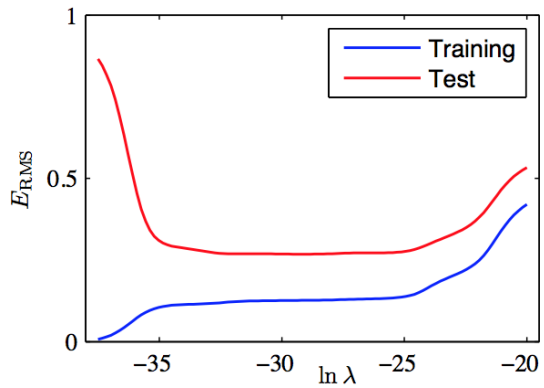


$\lambda = e^{-18}$



lambda $= 1$





	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
w_0	0.35	0.35	0.13
w_1	232.37	4.74	-0.05
w_2	-5321.83	-0.77	-0.06
w_3	48568.31	-31.97	-0.06
w_4	-231639.30	-3.89	-0.03
w_5	640042.26	55.28	-0.02
w_6	-1061800.52	41.32	-0.01
w_7	1042400.18	-45.95	-0.00
w_8	-557682.99	-91.53	0.00
w_9	125201.43	72.68	0.01

For a complex model ($M = 9$), training error increases with increasing regularization.

Linear Regression: To summarize

- **Representation:** linear and non-linear basis

  $f : \mathbf{x} \rightarrow y, \;\; f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$

  $f : \mathbf{z} \rightarrow y, \;\; f(\mathbf{x}) = \mathbf{w}^T\mathbf{z} = \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}), \;\; \boldsymbol{\phi} : \mathbf{x} \in \mathbb{R}^D \rightarrow \mathbf{z} \in \mathbb{R}^M$

- **Evaluation**: Minimizing residual sum of squares

  $\min_{\mathbf{w}} RSS(\mathbf{w}), \;\; RSS(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$

  $\min_{\mathbf{w}} RSS(\mathbf{w}), \;\; RSS(\mathbf{w}) = (\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})^T(\mathbf{y} - \boldsymbol{\Phi}\mathbf{w})$

- **Analytic Optimization**: Ordinary least squares (OLS) solution

  $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}, \;\; \mathbf{w}^* = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{y}$

- **Approximate Optimization**: Gradient descent (batch, stochastic, mini-batch)
- **Readings:** Alpaydin Ch 2, Abu-Mostafa Ch 3.2