Data Mining & Machine Learning

CS37300
Purdue University

Sep 27, 2023

Take-home Quiz

- Recall the previous example in the Decision Tree lecture

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

- Please construct a decision tree using information gain and full growth criteria.

Take-home Quiz

- Step 1. Compute the contingency table for each feature.

Age

	BC=yes	BC=no
<=30	2	3
31-40	4	0
>40	3	2

Income

	BC=yes	BC=no
High	2	2
Med	4	2
Low	3	1

Student

	BC=yes	BC=no
Yes	6	1
No	3	4

Credit

	BC=yes	BC=no
Fair	6	2
Excellent	3	3

Step 2. Compute the conditional probabilities $P(y|x_i=a)$.

Age

	BC=yes	BC=no
<=30	2/5	3/5
31-40	1	0
>40	3/5	2/5

Income

	BC=yes	BC=no
High	2/4	2/4
Med	4/6	2/6
Low	3/4	1/4

Student

	BC=yes	BC=no
Yes	6/7	1/7
No	3/7	4/7

Credit

	BC=yes	BC=no
Fair	6/8	2/8
Excellent	3/6	3/6

Take-home Quiz

- Compute the entropy and information gain for each feature at the root of the tree

$$Entropy(BC) = -\frac{5}{14}\log_2\frac{5}{14} - \frac{9}{14}\log_2\frac{9}{14} = 0.9403$$

Yes: 9
No: 5

Age

	BC=yes	BC=no
<=30	2/5	3/5
31-40	1	0
>40	3/5	2/5

$$Entropy(BC, age <= 30) = -\frac{2}{5}\log_2\frac{2}{5} - \frac{3}{5}\log_2\frac{3}{5} = 0.971$$

$$Entropy(BC, age = 31...40) = 0$$

$$Entropy(BC, age > 40) = -\frac{2}{5}\log_2\frac{2}{5} - \frac{3}{5}\log_2\frac{3}{5} = 0.971$$

$$Gain(BC, age) = 0.940 - \frac{5}{14}\cdot 0.971 - \frac{5}{14}\cdot 0.971 = 0.177$$

Take-home Quiz

- Compute the entropy and information gain for each feature at the root of the tree

$$Entropy(BC) = -\frac{5}{14}\log_2\frac{5}{14} - \frac{9}{14}\log_2\frac{9}{14} = 0.9403$$

Yes: 9
No: 5

Income

	BC=yes	BC=no
High	2/4	2/4
Med	4/6	2/6
Low	3/4	1/4

$$Entropy(BC, Income = high) = -\frac{2}{4}\log_2\frac{2}{4} - \frac{2}{4}\log_2\frac{2}{4} = 1$$

$$Entropy(BC, Income = medium) = -\frac{4}{6}\log_2\frac{4}{6} - \frac{2}{6}\log_2\frac{2}{6} = 0.918$$

$$Entropy(BC, Income = low) = -\frac{3}{4}\log_2\frac{1}{4} = 0.811$$

$$Gain(BC, Income) = 0.940 - (\frac{4}{14}\cdot 1 + \frac{6}{14}\cdot 0.918 + \frac{4}{14}\cdot 0.811) = 0.029$$

Take-home Quiz

- Compute the entropy and information gain for each feature at the root of the tree

$$Entropy(BC) = -\frac{5}{14}\log_2\frac{5}{14} - \frac{9}{14}\log_2\frac{9}{14} = 0.9403$$

Yes: 9
No: 5

student

	BC=yes	BC=no
Yes	6/7	1/7
No	3/7	4/7

$$Entropy(BC, student = no) = -\frac{3}{7}\log_2\frac{3}{7} - \frac{4}{7}\log_2\frac{4}{7} = 0.985$$

$$Entropy(BC, student = yes) = -\frac{6}{7}\log_2\frac{6}{7} - \frac{1}{7}\log_2\frac{1}{7} = 0.592$$

$$Gain(BC, student) = 0.940 - (\frac{7}{14}\cdot 0.985 + \frac{7}{14}\cdot 0.592) = 0.151$$

Take-home Quiz

- Compute the entropy and information gain for each feature at the root of the tree

$$Entropy(BC) = -\frac{5}{14}\log_2\frac{5}{14} - \frac{9}{14}\log_2\frac{9}{14} = 0.9403$$

Yes: 9
No: 5

Credit

	BC=yes	BC=no
Fair	6/8	2/8
Excellent	3/6	3/6

$$Entropy(BC, credit = fair) = -\frac{2}{8}\log_2\frac{2}{8} - \frac{6}{8}\log_2\frac{6}{8} = 0.811$$

$$Entropy(BC, credit = excellent) = -\frac{3}{6}\log_2\frac{3}{6} - \frac{3}{6}\log_2\frac{3}{6} = 1$$

$$Gain(BC, credit) = 0.940 - (\frac{8}{14}\cdot 0.811 + \frac{6}{14}\cdot 1) = 0.048$$

Take-home Quiz

- Pick the feature with the largest information gain

$$Gain(BC, age) = 0.940 - \frac{5}{14} \cdot 0.971 - \frac{5}{14} \cdot 0.971 = 0.177$$

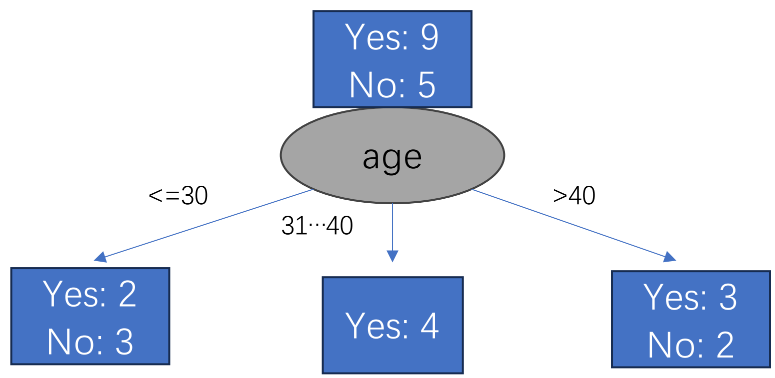
$$Gain(BC, Income) = 0.940 - (\frac{4}{14} \cdot 1 + \frac{6}{14} \cdot 0.918 + \frac{4}{14} \cdot 0.811) = 0.029$$

$$Gain(BC, student) = 0.940 - (\frac{7}{14} \cdot 0.985 + \frac{7}{14} \cdot 0.592) = 0.151$$

$$Gain(BC, credit) = 0.940 - (\frac{8}{14} \cdot 0.811 + \frac{6}{14} \cdot 1) = 0.048$$

Take-home Quiz

- Partition the initial dataset based on age and grow the tree by one level



Take-home Quiz

- The first subset is not a “pure” (i.e. entropy = 0) set, continue to partition it.
- Repeat the previous steps on the first subset

Income

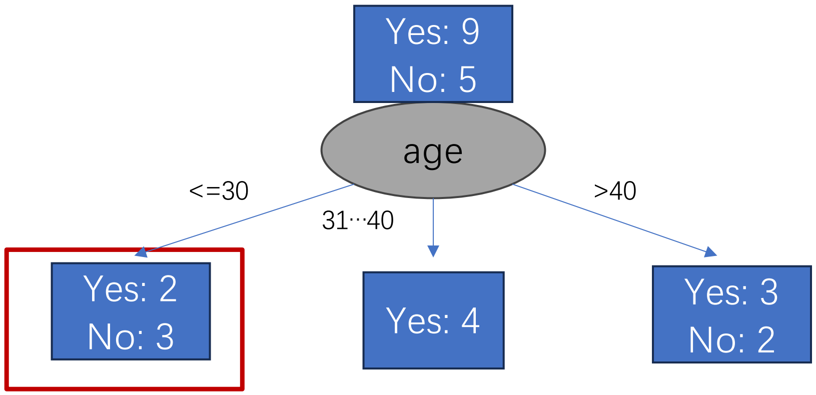
	BC=yes	BC=no
High	0	2
Med	1	1
Low	1	0

Student

	BC=yes	BC=no
Yes	2	0
No	0	3

Credit

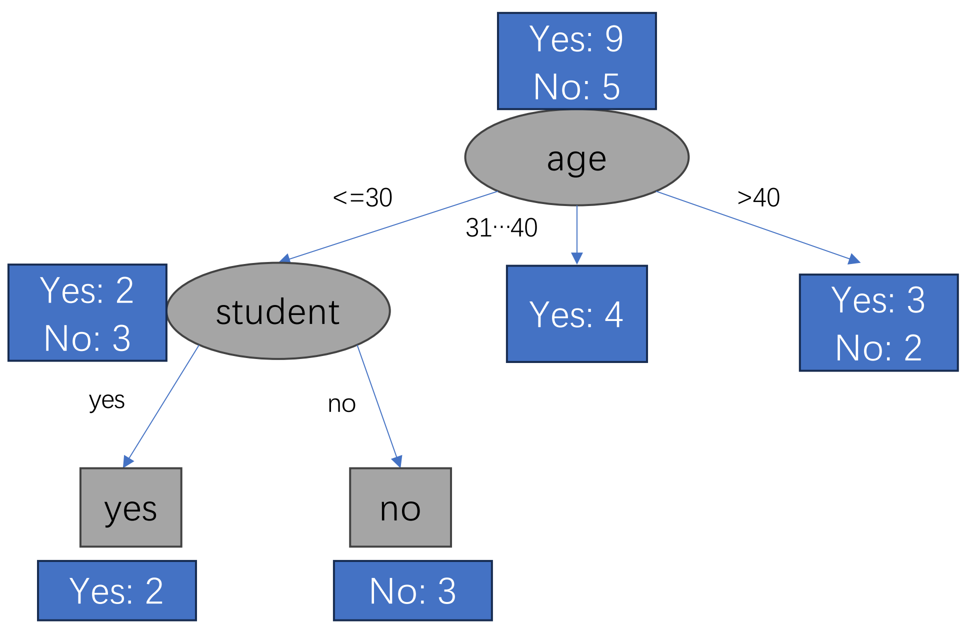
	BC=yes	BC=no
Fair	1	2
Excellent	1	1



No need to further calculate. We already see a feature that splits the first subset to two pure sets.

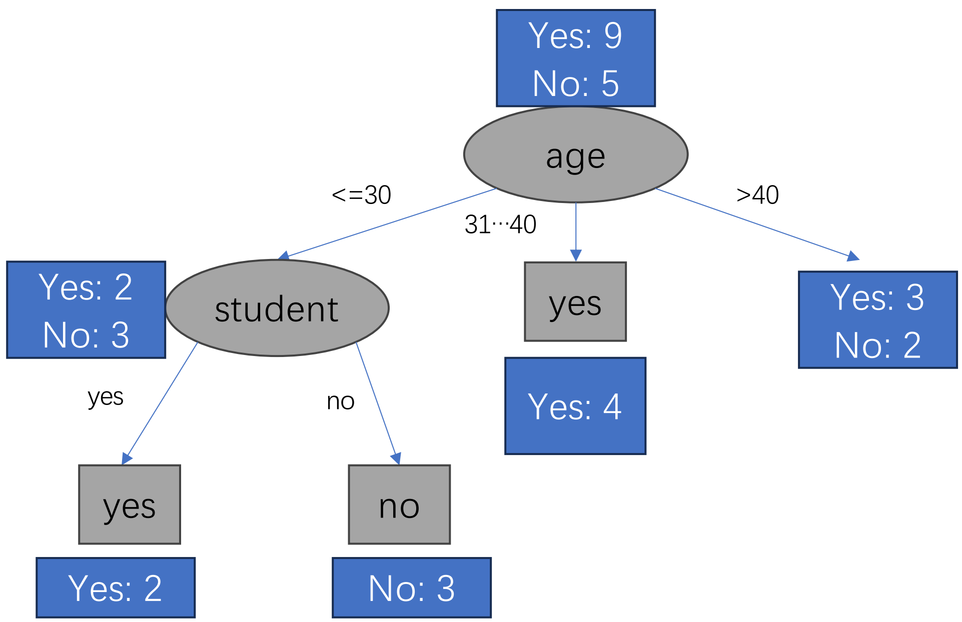
Take-home Quiz

- Spit the first subset based on the student feature



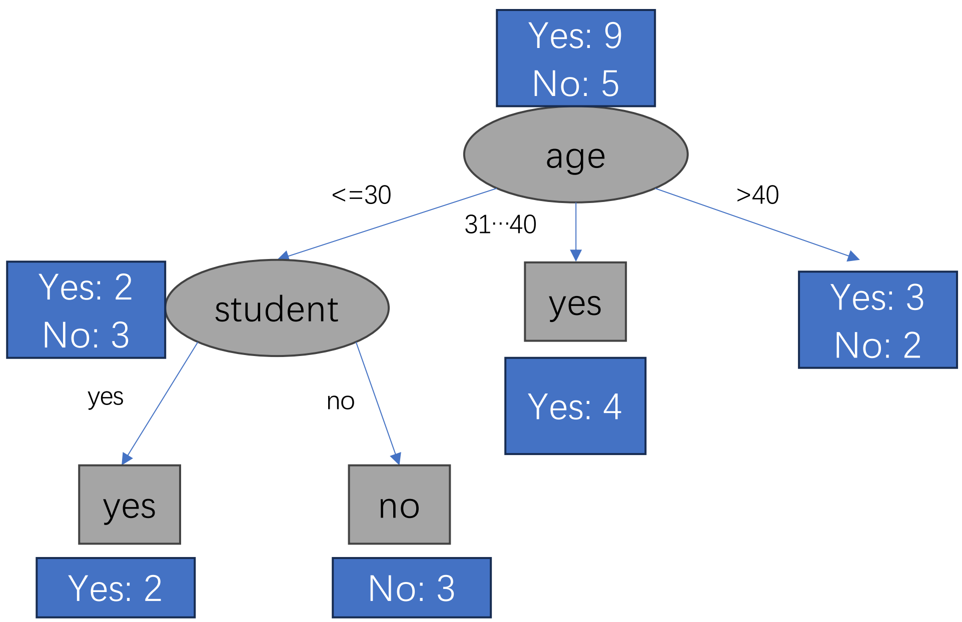
Take-home Quiz

- The second subset at Depth 1 is already a “pure” set
- No need to further partition



Take-home Quiz

- The third subset at Depth 1 is not a “pure” set
- Need to further partition. Repeat previous steps.



Take-home Quiz

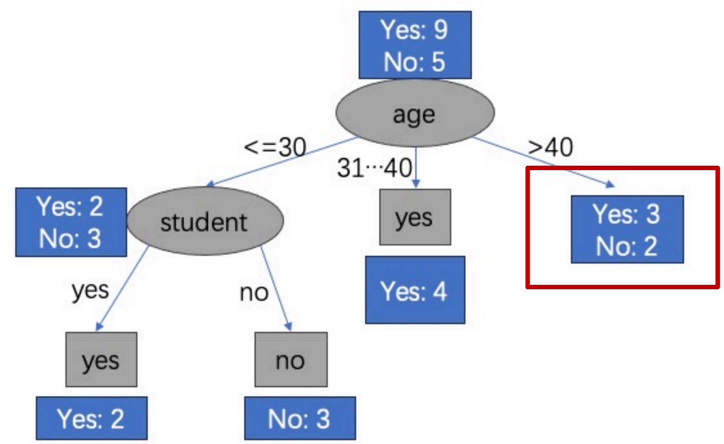
- The third subset at Depth 1 is not a pure set
- Need to further partition. Repeat previous steps.

Income

	BC=yes	BC=no
High	0	0
Med	2	1
Low	1	1

Student

	BC=yes	BC=no
Yes	2	1
No	1	1



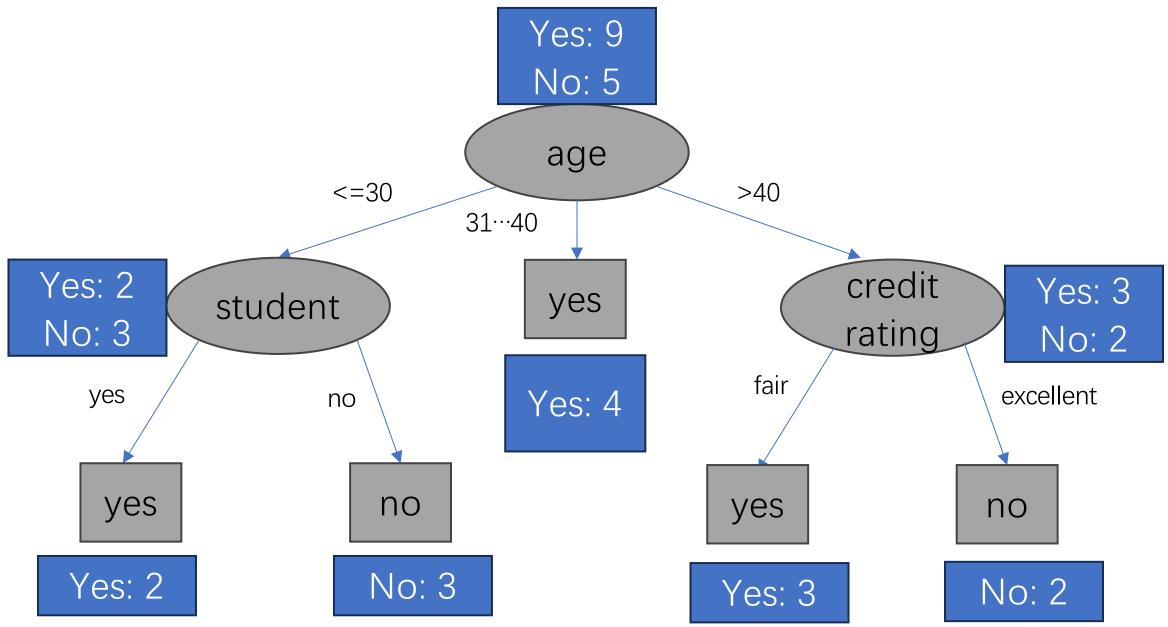
Credit

	BC=yes	BC=no
Fair	3	0
Excellent	0	2

No need to further calculate. We already see a feature that splits the first subset to two pure sets.

Take-home Quiz

- Spit the third subset based on the credit feature



Today’s topics

- Gradient descent (contd)
- Linear regression

Gradient descent

Convex optimization problems

$$\begin{array}{rl} \text{minimize} & f(x) \\ \text{subject to} & x \in C \end{array}$$

- *x* is the optimization variable (*e.g., model parameters*)
  f (*e.g., score function*) is a **convex function**
  C is a **convex set** (*e.g., constraints on model parameters*)

- For convex optimization problems, all locally optimal points are globally optimal

Solve convex optimization problem

- Minimize a convex function without any constraints on the variables
  - If f'(x)=0 then x is a stationary point of f
  - If f'(x)=0 and f''(x) is not negative then x is a local minimum of f (for convex function, this is also a global minimum)
  - If f is a strictly convex function, any stationary point of ***f*** is the unique global minimum of f

Gradient descent

- For some convex functions, we may be able to take the derivative, but it may be difficult to directly solve for parameter values
- Solution:
  - Start at some value of the parameters
  - Take derivative and use it to move the parameters in the direction of the negative gradient
  - Repeat until stopping criteria is met (e.g., gradient close to 0)

<u>Gradient Descent Rule:</u>

$$\underline{\mathbf{w}}_{\mathbf{new}} = \underline{\mathbf{w}}_{\mathbf{old}} - \eta \ \Delta\,(\underline{\mathbf{w}})$$

where

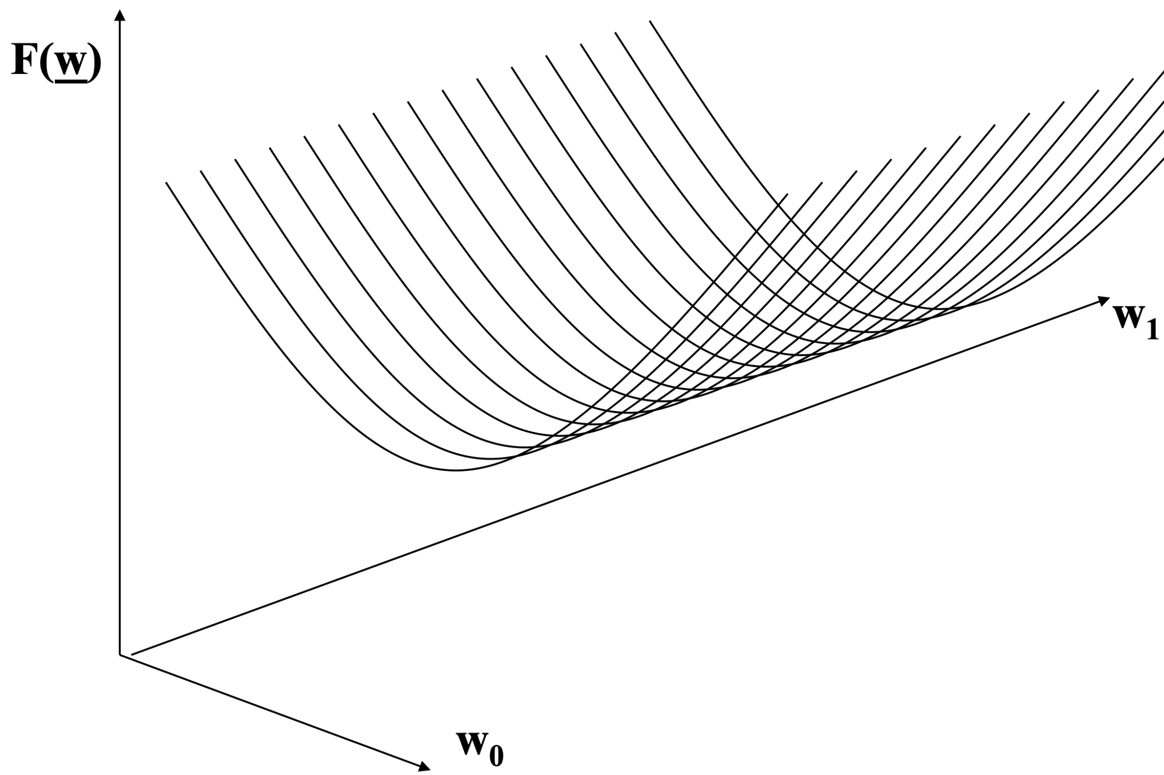
$\Delta\,(\underline{w})$ is the gradient and

η is the learning rate (small, positive)

Notes:

1. This moves us downhill in direction $\Delta\,(\underline{\mathbf{w}})$ (steepest downhill direction)
2. How far we go is determined by the value of η

Illustration of gradient descent



Slides adapted from CS175, UCIrvine, Padhraic Smyth

Illustration of gradient descent

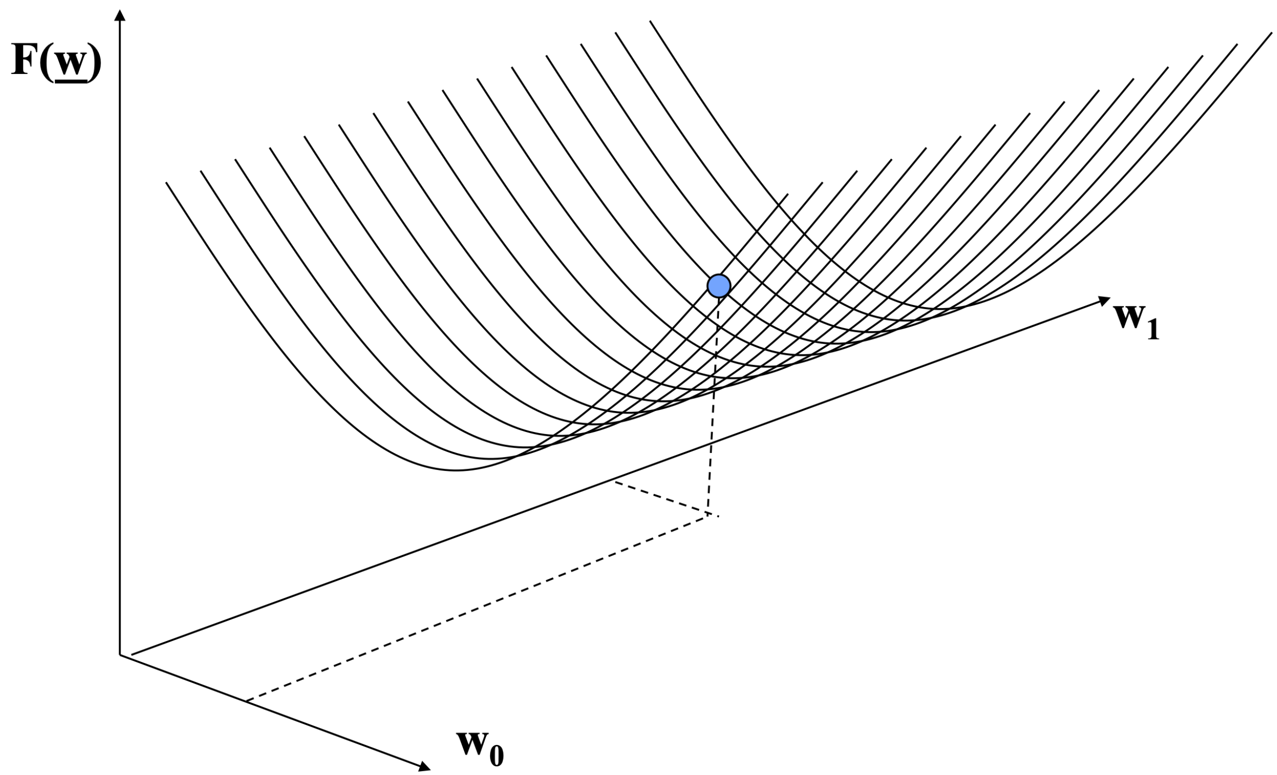


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Illustration of gradient descent

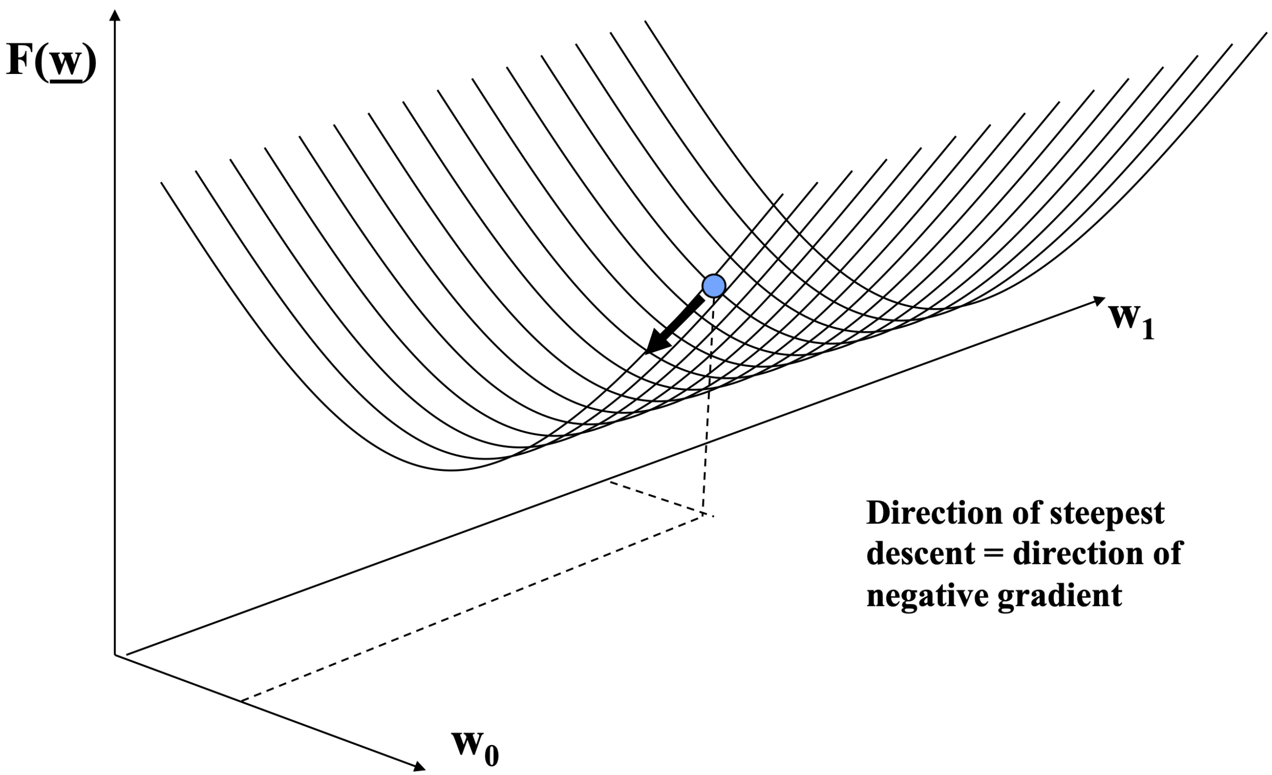

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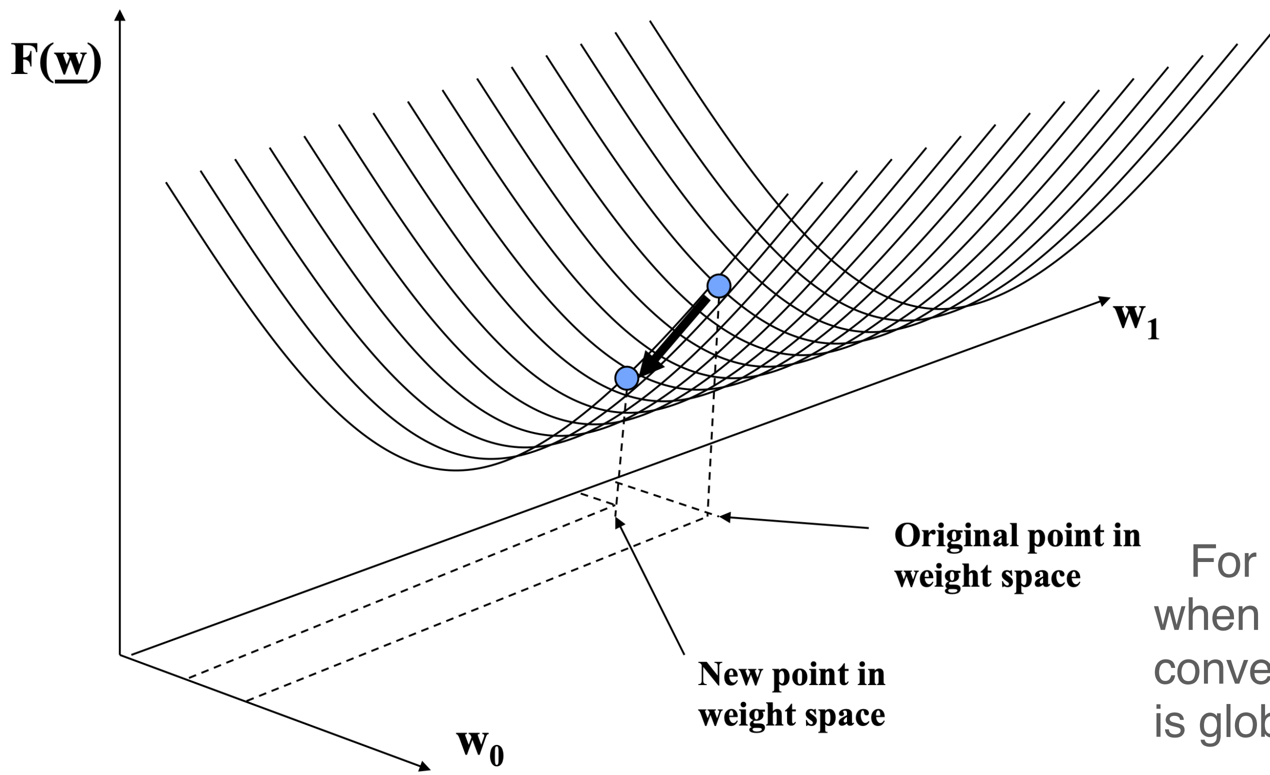
Illustration of gradient descent



For convex functions, when gradient descent converges, the solution is global minimum.

Slides adapted from CS175, UCIrvine, Padhraic Smyth

Stopping criteria

- Ideally, f'(x)=0…
- In practice…
  - $\| \nabla f(x) \| < \varepsilon$
  - $|f(x_{k+1}) - f(x_k)| < \varepsilon$
  - $\| x_{k+1} - x_k \| < \varepsilon$
  - Maximum number of iterations has been reached

Extensions

- “Higher” order methods
    - Approximate higher order methods
- Constrained optimization
- Accelerated optimization
- Stochastic optimization
- Online setting

Stochastic Gradient descent

- Sample data points (say uniformly at random)
- Use only the gradients on the sampled “batch”
- Lower per-iteration cost
- Usually higher number of iterations
- Is NOT a ”descent” algorithm
- Can possibly help escape local minima (better for non-convex functions)

Analysis

- What is space and time complexity of a single iteration of gradient descent for a *separable* loss function (separable on data points, NOT in context of margin here)?
    - Assume cost of calculating the gradient is g, total number of data points is n
- How many iterations?
    - Second order vs first order
    - Stochastic vs Deterministic
- Total cost associated with the algorithm is sum of the above costs.
- Except for constrained optimization, which may have a “projection” cost associated

Linear Regression

Setup

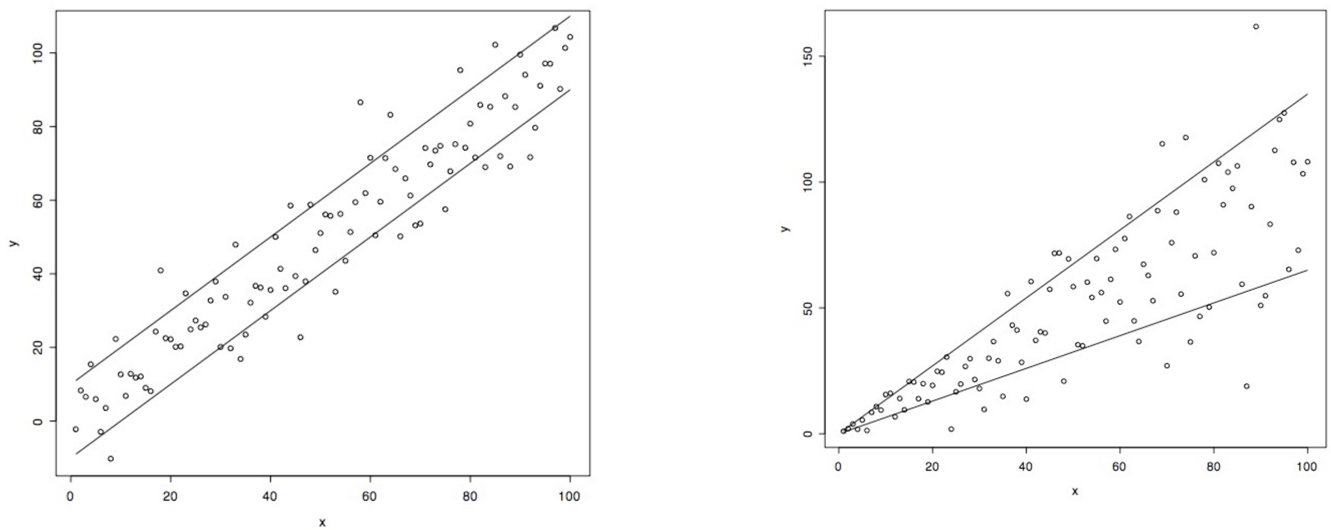
- Data $\{x_i, y_i\}$ Total *n* data points, $x_i \in R^d, y \in R$.
- $y \sim w^\top x$
- Cost function:
  - $\min_w \sum_i \quad |y_i \, - w^\top x_i|$^2

Closed form solution

- $w^{\star} = (X^T X)^{-1} X^T y$
- Prediction: $w^{\star T} x_{test}$
- What is the time and space complexity ?
- What if $X^{\top} X$ is not invertible? When does this happen?

Probabilistic interpretation

- $y = x^{\top}w + \epsilon$, where $\epsilon \sim N(0, \sigma^2)$
- MLE in this model is equivalent to linear regression
- Clearly delineates the underlying "implicit" assumptions in the least squared loss e.g. Homoskedasticity.



- Probabilistic interpretation also quantifies uncertainty under the same assumptions

Generalized Linear Models (GLMs)

- Y is a RV from a distribution in the exponential family e.g. Gaussian, Bernoulli, Poisson etc
- For some function $g()$
  - $g(E[Y]) = (x^T w)$
- Allows for certain algorithms to be applied widely to all GLMs.