CX4240 Spring 2026

Supervised Learning: Linear Regression

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Organization

- ***Background knowledge***
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills (PyTorch and JAX)
- ***Supervised learning***
- ***Unsupervised learning***
- ***Advanced Topics***

Syllabus

- ***Background knowledge***
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- ***Supervised learning***
- ***Unsupervised learning***
- ***Advanced Topics: LLM & RL***

}

Modeling: what to learn

Learning: how to learn

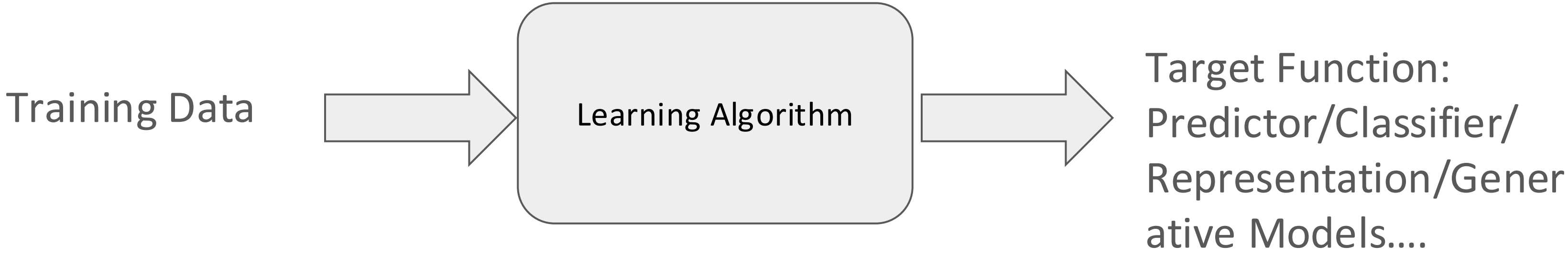
Implementation

Syllabus

- ***Background knowledge***
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- ***Supervised learning***
- ***Unsupervised learning***
- ***Advanced Topics: LLM & RL***

Modeling: Probability and Statistics, Linear Algebra
Learning: Optimization, Linear Algebra
Implementation: Coding (PyTorch/JAX)

ML Algorithm Pipeline

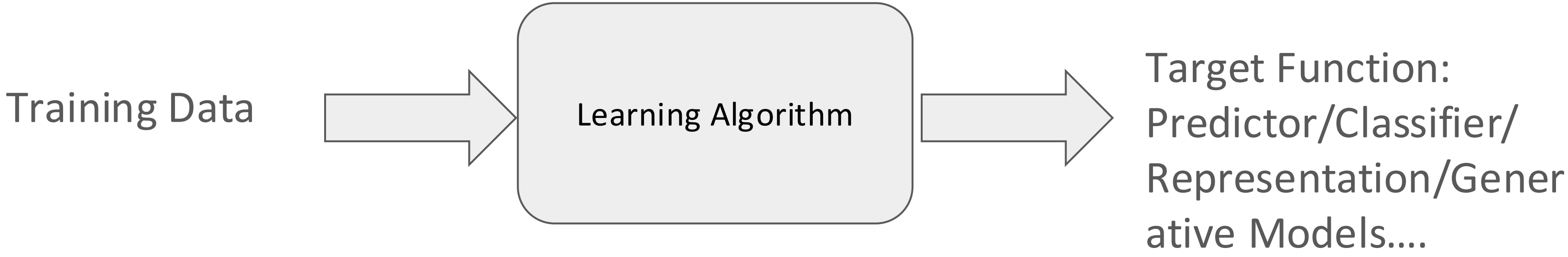


Training Data

Learning Algorithm

Target Function: Predictor/Classifier/ Representation/Generative Models….

ML Algorithm Pipeline



Training Data

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Target Function: Predictor/Classifier/Representation/Generative Models....

General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE/MAP, maximum margin, contrastive…)
3. Select optimizer

Syllabus

- ***Background knowledge***
  - Probability and Statistics, Linear Algebra, Optimization, Coding skills
- ***Supervised learning***
- ***Unsupervised learning***
- ***Advanced Topics***

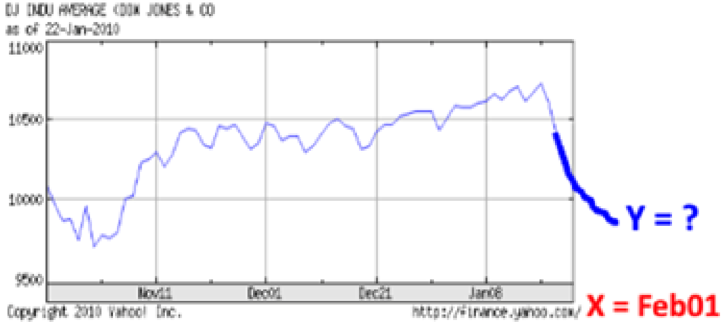
Modeling: Probability and Statistics, Linear Algebra
Learning: Optimization, Linear Algebra
Implementation: Coding

Supervised Learning

Goal: Construct a **predictor** f: X → Y

→ Sports
Science
News

**Classification:
discrete categories**

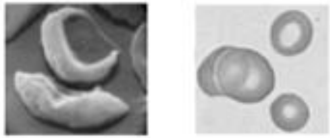


**Regression:
Real-valued numbers**

Classification Tasks

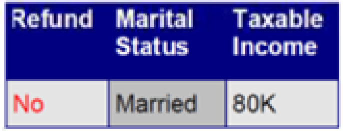
	Feature, X	Label, Y

Diagnosing sickle cell anemia

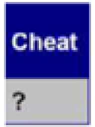


Anemic cell
Healthy cell

Tax Fraud Detection



Refund	Marital Status	Taxable Income
No	Married	80K



Cheat
?

Web Classification

Sports
Science
News

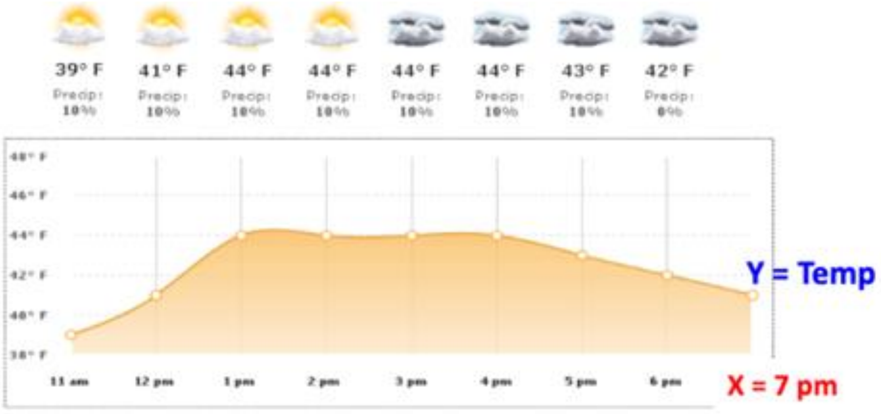
Predict Fulton resident

Drive to GT, Hawk's fan, Shop at Publix

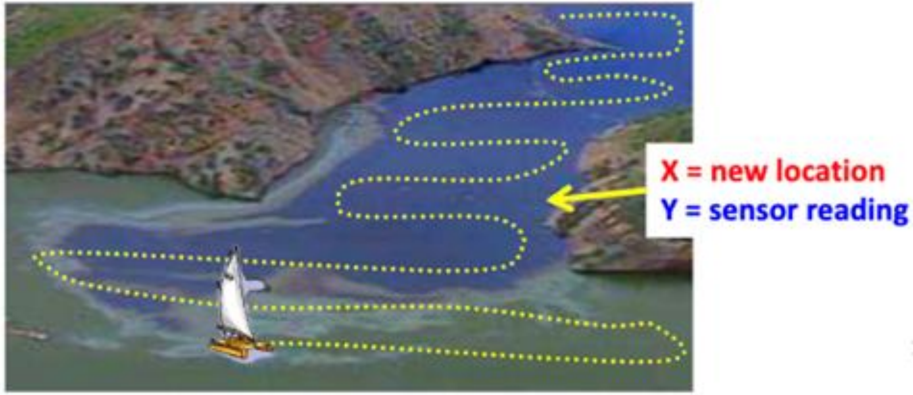
Resident
Not resident

Regression Tasks

Weather Prediction



Estimating Contamination

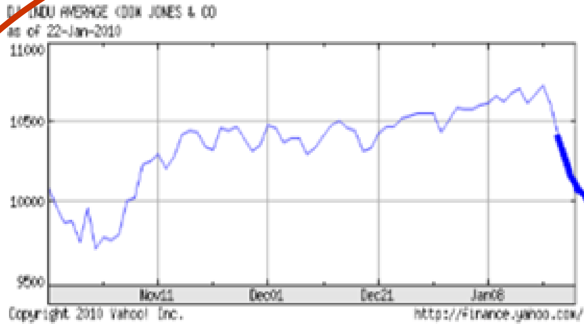


Supervised Learning

Goal: Construct a **predictor** f: X → Y to
minimize a risk (performance measure) R(f).

Sports
Science
News

Classification:
discrete categories

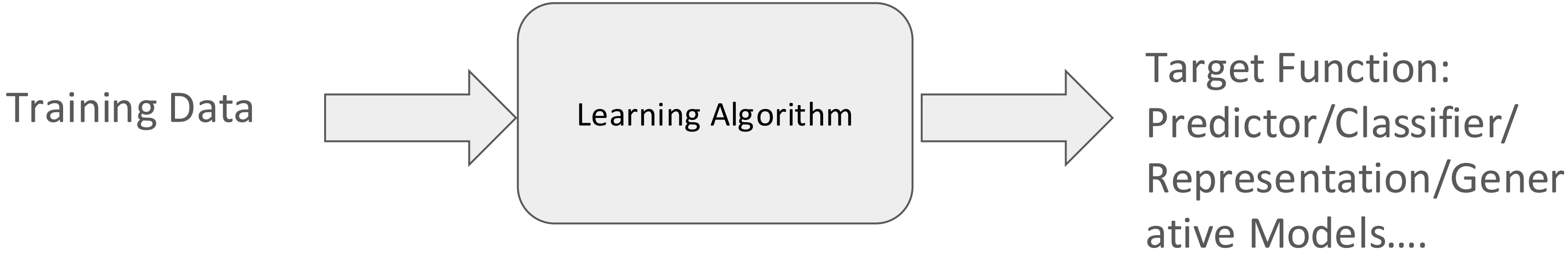


Y = ?

X = Feb01

Regression:
Real-valued number

ML Algorithm Pipeline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General ML Algorithm Pipeline

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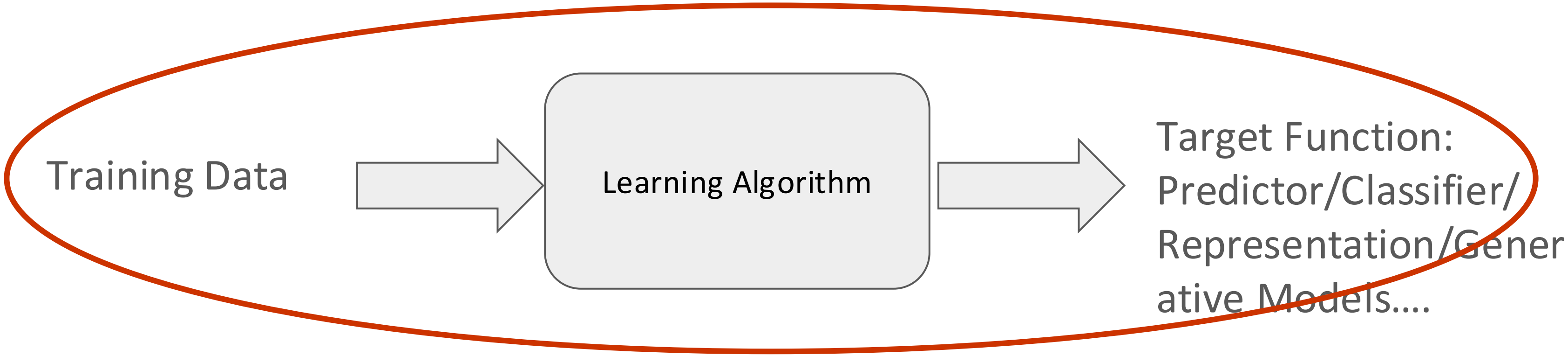
ML Algorithm Pipeline



General ML Algorithm Pipeline

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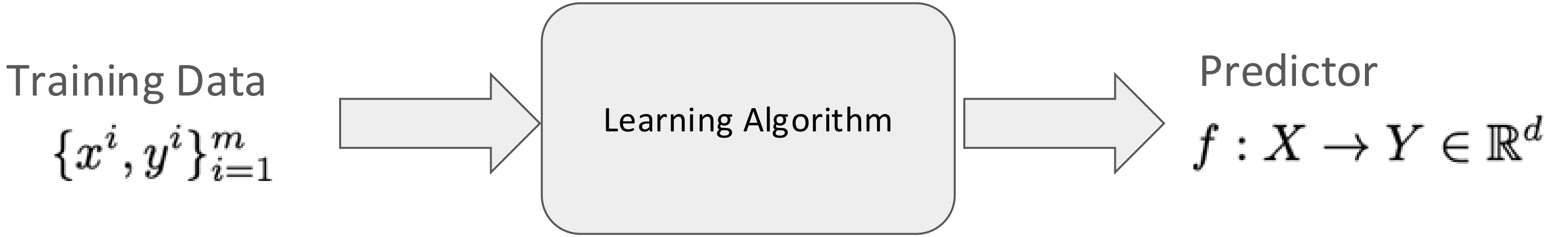
Machine Learning for Apartment Hunting

- Suppose you are to move to Atlanta
- And you want to find the most reasonably priced apartment satisfying your needs:

X y

Living area (ft^2)	# bedroom	Monthly rent ($)
230	1	900
506	2	1800
433	2	1500
190	1	800
...		
150	1	?
270	1.5	?

Regression algorithms



Training Data

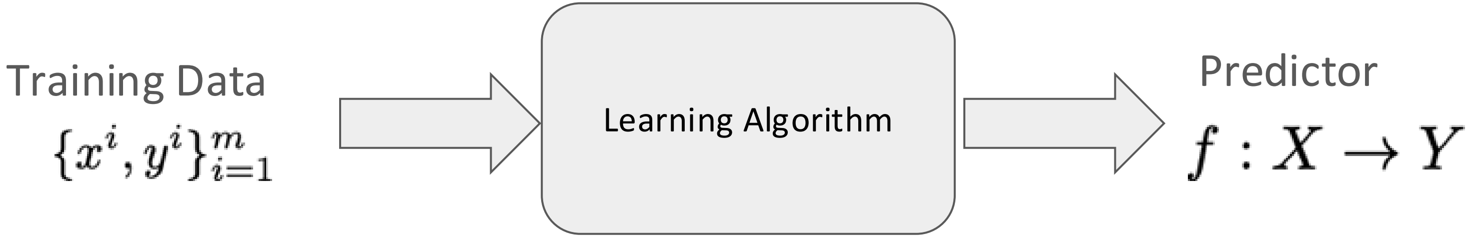
$\{x^i, y^i\}_{i=1}^m$

Learning Algorithm

Predictor

$f : X \to Y \in \mathbb{R}^d$

Regression algorithms



Training Data

$\{x^i, y^i\}_{i=1}^m$

Learning Algorithm

Predictor

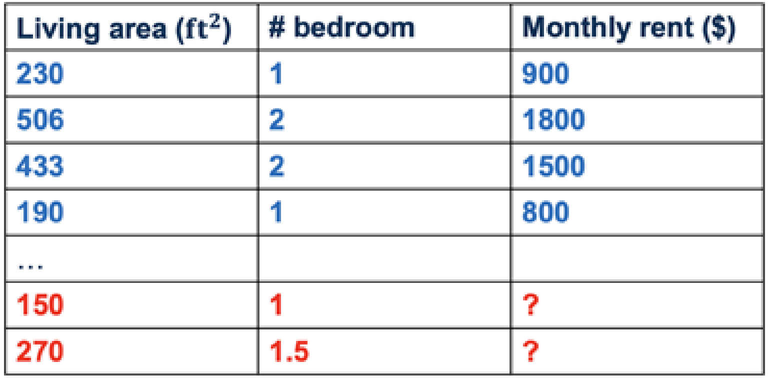
$f : X \to Y$

- **Features:**
  - Living area, distance to campus, # of bedroom …
  - Denotes as $x = (x_1, x_2, \ldots, x_n)^\top$
- **Target**
  - Rent
  - Denote as y
- **Training set**

  $X = (x^1, x^2, \ldots, x^m)$

  $y = (y^1, y^2, \ldots, y^m)^\top$

$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$$



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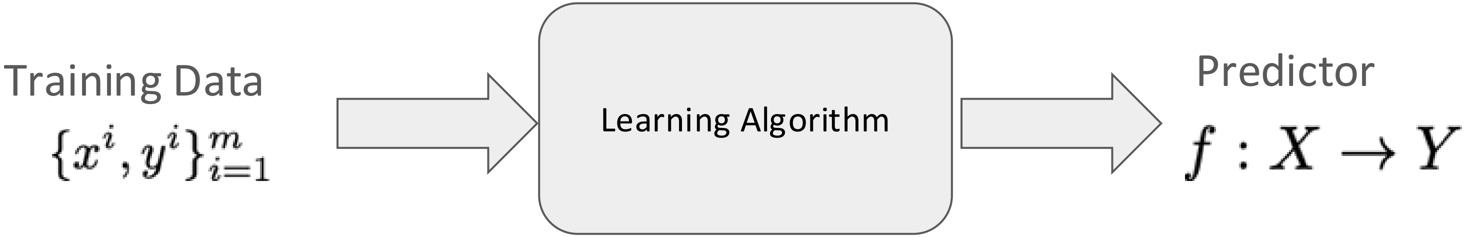

General ML Algorithm Pipeline

1. Build probabilistic models
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Probabilistic Model:
Linear Regression Model with Gaussian Noise

- Assume y is a linear function of x (features) plus noise ϵ

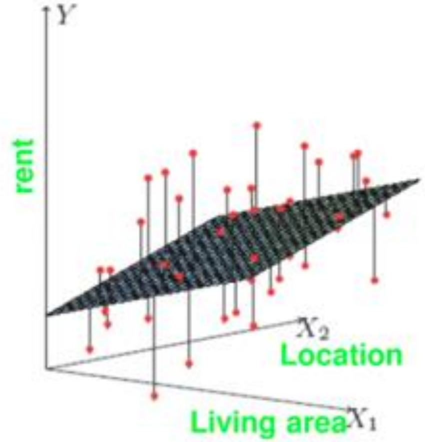
$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n + \epsilon$$

where ϵ is an error model as Gaussian $N(0, \sigma^2)$

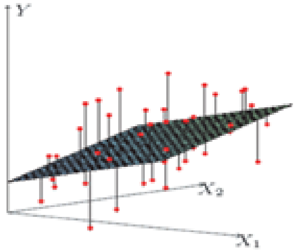
- Let $\theta = (\theta_0, \theta_1, \ldots, \theta_n)^\top$, and augment data by one dimension

$$x \leftarrow (1, x)^\top$$

Then $y = \theta^\top x + \epsilon$



Probabilistic Model: Gaussian Likelihood

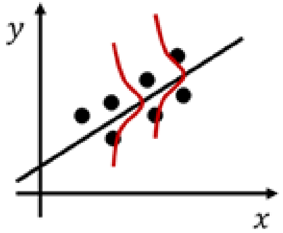


- Assume y is a linear in x plus noise ϵ

$$y = \theta^\top x + \epsilon$$

- Assume ϵ follows a Gaussian $N(0, \sigma)$

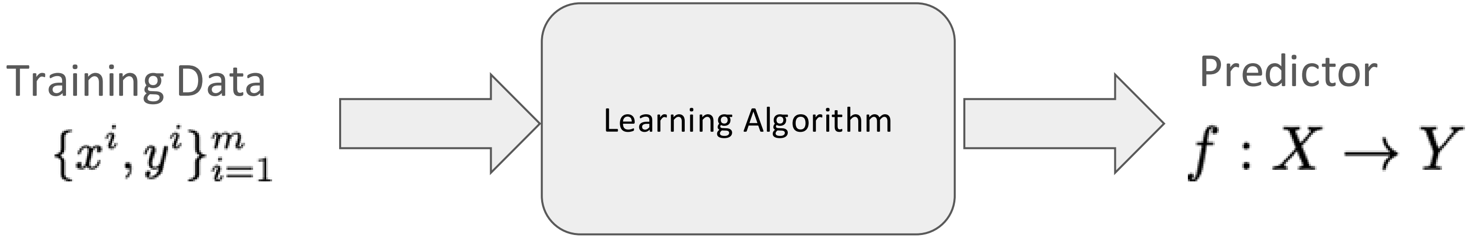
$$p(y^i \mid x^i; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$



- By independence assumption, likelihood is

$$L(\theta) = \prod_i^m p(y^i \mid x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Regression algorithms



Training Data

$\{x^i, y^i\}_{i=1}^m$

Learning Algorithm

Predictor

$f : X \rightarrow Y$

General ML Algorithm Pipeline

1. Build probabilistic models
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3. Select optimizer

Maximum log-Likelihood Estimation (MLE)

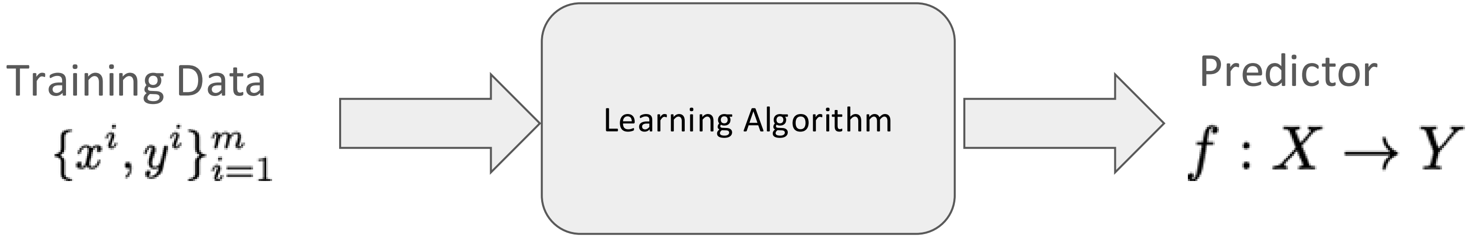
$$L(\theta) \;= \prod_{i}^{m} p(y^i|x^i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Maximum log-Likelihood Estimation (MLE)

$$L(\theta) \; = \prod_{i}^{m} p(y^i | x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$

$$\max_{\theta} \; \log L(\theta) = -\frac{1}{2\sigma^2} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2 - m \log(\sqrt{2\pi}\sigma)$$

Regression algorithms



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$f : X \to Y$

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Select Optimizer

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

Select Optimizer

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

- Necessary Condition
- (Stochastic) Gradient Descent

Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} \qquad\qquad\qquad\qquad = 0$$

Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i) x^{i\top} = 0$$

Necessary Condition

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^{i\top} = 0$$

$$\Leftrightarrow -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i x^{i\top}\theta = 0$$

Necessary Condition

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i {x^i}^\top \theta = 0$$

Necessary Condition

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i {x^i}^\top \theta = 0$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}(x^1 \dots, x^m)(y^1 \dots, y^m)^\top + \frac{2}{m}(x^1, \dots x^m)(x^1, \dots x^m)^\top \theta = 0$$

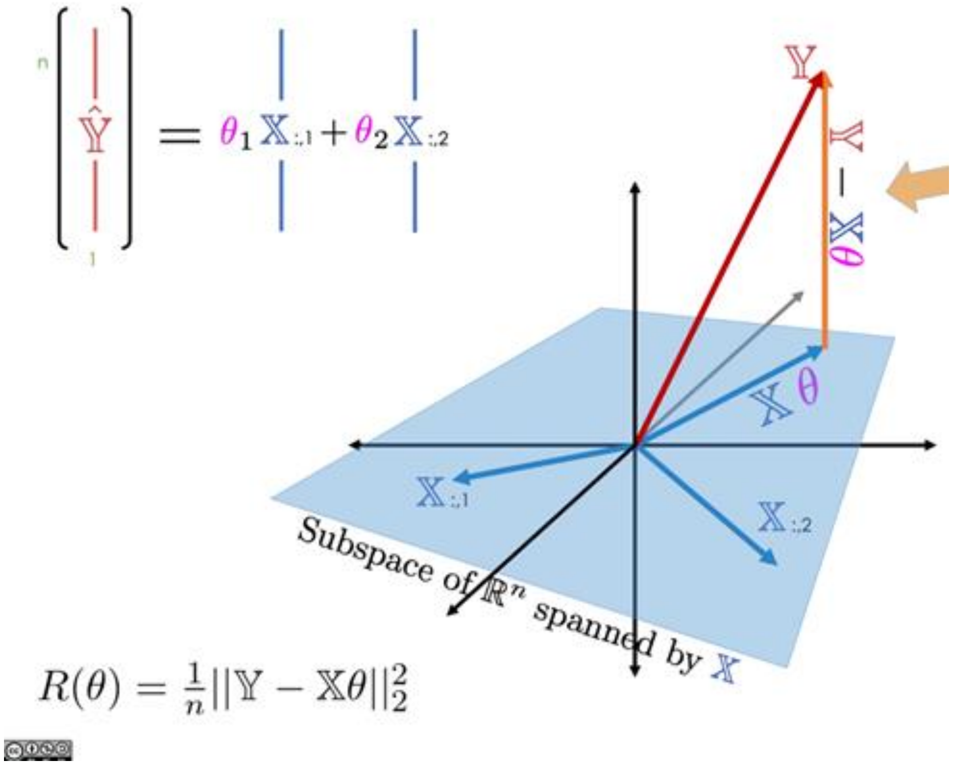
Define $X = (x^1, x^2, \dots x^m), y = (y^1, y^2, \dots, y^m)^\top$, gradient becomes

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m} Xy + \frac{2}{m} XX^\top \theta = 0$$

$$\Rightarrow \hat{\theta} = (XX^\top)^{-1} Xy$$

Geometric Interpretation

$$\hat{\theta} = (XX^{\top})^{-1}Xy$$



$$\hat{\mathbb{Y}} = \theta_1 \mathbb{X}_{:,1} + \theta_2 \mathbb{X}_{:,2}$$

$$R(\theta) = \frac{1}{n}||\mathbb{Y} - \mathbb{X}\theta||_2^2$$

n
1
$\mathbb{Y}$
$\mathbb{Y} - \mathbb{X}\theta$
$\mathbb{X}\theta$
$\mathbb{X}_{:,1}$
$\mathbb{X}_{:,2}$
Subspace of $\mathbb{R}^n$ spanned by $\mathbb{X}$

Select Optimizer

$$\min_{\theta} \; -\log L(\theta) \propto \frac{1}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2$$

- Necessary Condition
- (Stochastic) Gradient Descent

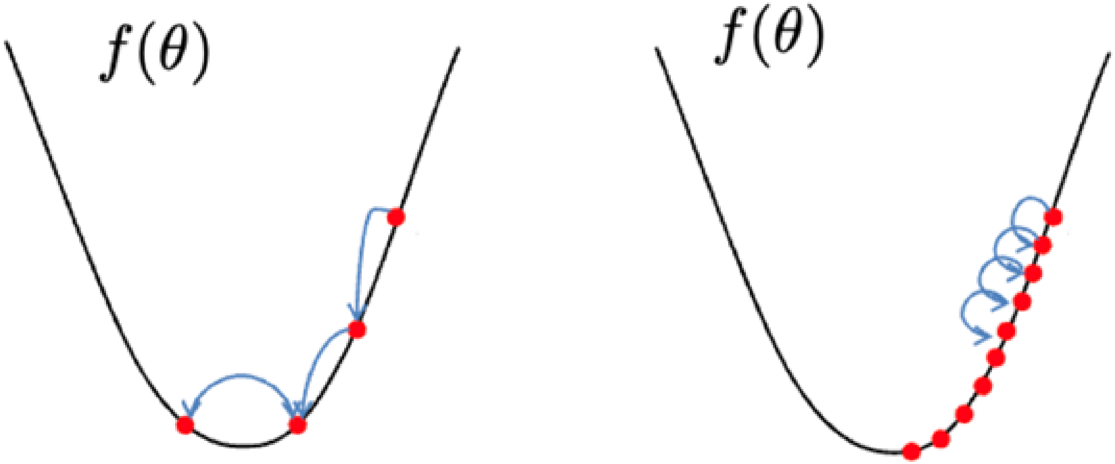
Gradient Method Revisit

$$\min_{\theta} \; \underbrace{-\log L(\theta) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2}_{f(\theta)}$$

choose an initial $\theta^1 \in \mathbf{R}^d$ and $h^1 > 0$ (e.g., $\theta^1 = 0, h^1 = 1$)
for $k = 1,2,\ldots,k^{\max}$

1. compute $\nabla f(\theta^k)$; quit if $\|\nabla f(\theta^k)\|_2$ is small enough
2. form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$
3. if $f(\theta^{\text{tent}}) < f(\theta^k)$, set $\theta^{k+1} = \theta^{\text{tent}}, h^{k+1} = 1.2h^k$
4. else set $h^k := 0.5h^k$ and go to step 2

Effect of Learning Rate in GD



Large α ⇒ Fast convergence but larger residual error. Also possible oscillation.
Small α ⇒ Slow convergence but small residual error.

Gradient Calculation

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^i$$

form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$

$$\theta^k + \frac{h^k}{m}\sum_{i=1}^{m}(y^i - (\theta^k)^\top x^i)(x^i)^\top$$

Gradient Method Revisit

```
choose an initial $\theta^1 \in \mathbf{R}^d$ and $h^1 > 0$ (e.g., $\theta^1 = 0, h^1 = 1$ )
for $k = 1,2,\dots,k^{\text{max}}$
                    Stochastic Approximation
    1.  compute $\nabla \cancel{f(\theta^k)}$; quit if $\|\nabla f(\theta^k)\|_2$ is small enough
    2.  form tentative update $\theta^{\text{tent}} = \theta^k - h^k \nabla f(\theta^k)$
    3.  if $f(\theta^{\text{tent}}) < f(\theta^k)$, set $\theta^{k+1} = \theta^{\text{tent}}, h^{k+1} = 1.2h^k$
    4.  else set $h^k := 0.5h^k$ and go to step 2
```

Stochastic Gradient Descent

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^i \quad \approx \quad \left(y^i - \hat{\theta}^{t\top} x^i\right) x^i$$

Initialize $\theta^0 \in \mathbb{R}^d$ randomly Iterate until convergence:

1 Randomly sample a point (x_i, y_i) from the n data points

2 Compute noisy gradient $\tilde{g}^t = (y^i - (\theta^t)^\top x^i)(x^i)^\top$

3 Update (GD): $\theta^{t+1} = \theta^t - \eta \tilde{g}^t$

Recap

- Stochastic gradient update rule

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \beta \left(y^{i} - (\hat{\theta}^{t})^{\top} x^{i} \right) x^{i}$$

  - Pros: online, low per-step cost
  - Cons: coordinate, (sometimes) slow-converging
- Gradient descent

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \frac{\alpha}{m} \sum_{i=1}^{m} \left(y^{i} - (\hat{\theta}^{t})^{\top} x^{i} \right) x^{i}$$

  - Pros: fast-converging, easy to implement
  - Cons: need to read all data
- Solve normal equations

$$(X^{\top} X)\hat{\theta} = X^{\top} y$$

  - Pros: a single-shot algorithm! Easiest to implement
  - Cons: need to compute inverse, expensive, numerical issue (e.g., matrix is singular …)

Summary

General ML Algorithm Pipeline

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2. Derive loss function (by MLE or MAP)
3. Select optimizer

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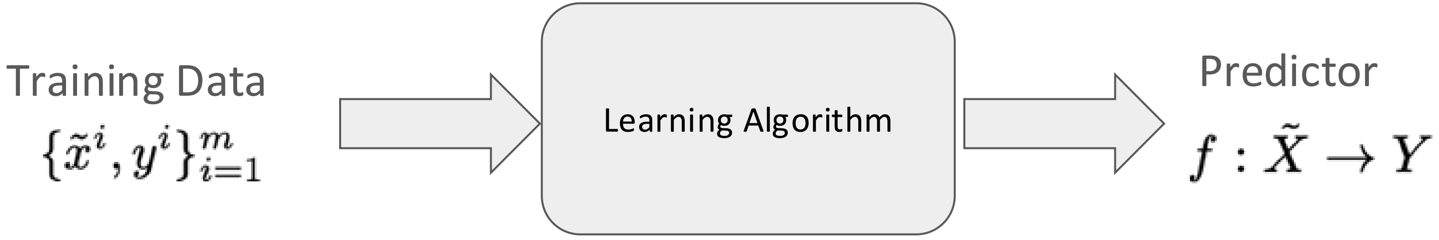
Polynomial Regression



Training Data

$\{\tilde{x}^i, y^i\}_{i=1}^{m}$

Learning Algorithm

Predictor

$f : \tilde{X} \to Y$

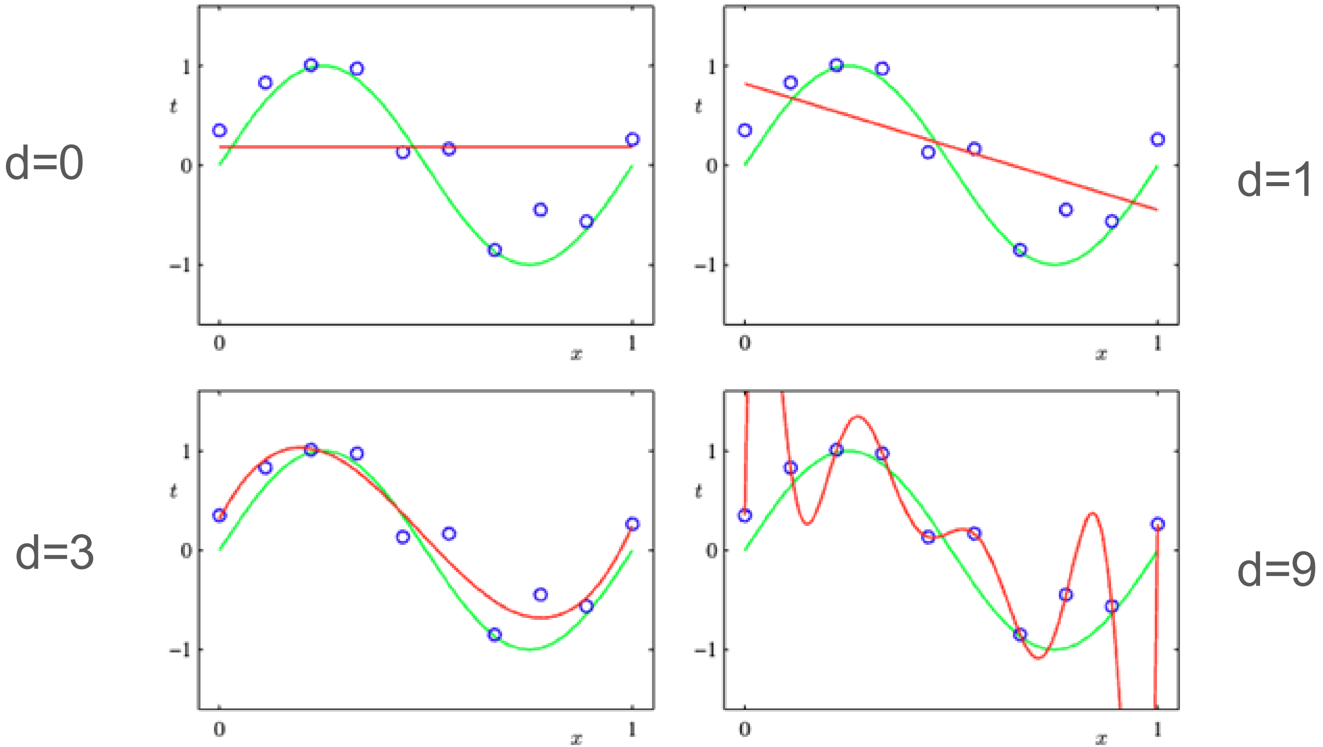
$$
\begin{aligned}
y = \theta_0 &+ \theta_1^1 x_1 + \theta_1^2 (x_1)^2 + \theta_1^3 (x_1)^3 + \ldots + \theta_1^d (x_1)^d \\
&+ \theta_2^1 x_2 + \theta_2^2 (x_2)^2 + \theta_2^3 (x_2)^3 + \ldots + \theta_2^d (x_2)^d \\
&+ \ldots \\
&+ \theta_n^1 x_n + \theta_n^2 (x_n)^2 + \theta_n^3 (x_n)^3 + \ldots + \theta_n^d (x_n)^d
\end{aligned}
$$

- **Features:**
  - Living area, distance to campus, # of bedroom …
  - Denotes as $\tilde{x} = [1, x_1, (x_1)^2, \ldots, (x_1)^d, \ldots, x_n, \ldots, (x_n)^d]$
- **Target**
  - Rent
  - Denote as y
- **Training set**

  $\tilde{X} = [\tilde{x}^1, \tilde{x}^2, \ldots, \tilde{x}^m]$

  $y = (y^1, y^2, \ldots, y^m)^\top$

Overfitting with Increased Degree



Summary

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1. Build probabilistic models
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Maximum a Posteriori (MAP)

$$L(\theta) \;= \prod_{i}^{m} p(y^i | x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$ Likelihood

$$p(\theta) \propto \exp(-\lambda \|\theta\|^2)$$ Gaussian Prior

Maximum a Posteriori (MAP)

$$L(\theta) \ = \prod_{i}^{m} p(y^i|x^i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\sum_i^m \left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda\|\theta\|_2^2)$$

Gaussian Prior

$$p(\theta|\{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i|x^i,\theta)p(\theta)}{\int \prod_{i=1}^m p(y^i|x^i,\theta)p(\theta)d\theta}$$

Posterior: Bayes' Rule

Maximum a Posteriori (MAP)

$$L(\theta) \ = \prod_{i}^{m} p(y^i|x^i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\Sigma_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda \|\theta\|_2^2)$$

Gaussian Prior

$$p(\theta|\{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i|x^i,\theta)p(\theta)}{\int \prod_{i=1}^m p(y^i|x^i,\theta)p(\theta)d\theta}$$

Posterior: Bayes' Rule

$$\max_{\theta} \ \log p(\theta|\{x^i, y^i\}_{i=1}^m)$$

MAP

Maximum a Posteriori (MAP)

$$L(\theta) = \prod_{i}^{m} p(y^i|x^i;\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\Sigma_i^m\left(y^i - \theta^\top x^i\right)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda\|\theta\|_2^2)$$

Gaussian Prior

$$p(\theta|\{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i|x^i,\theta)p(\theta)}{\int \prod_{i=1}^m p(y^i|x^i,\theta)p(\theta)d\theta}$$

Posterior: Bayes' Rule

$$\max_\theta \; \log p(\theta|\{x^i, y^i\}_{i=1}^m) = \log L(\theta) + \log p(\theta)$$

Ridge Regression

$$\propto -\frac{1}{m}\sum_{i=1}^m (y^i - \theta^\top x^i)^2 - \lambda\|\theta\|_2^2$$

Maximum a Posteriori (MAP)

$$L(\theta) = \prod_{i}^{m} p(y^i | x^i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^m \exp\left(-\frac{\Sigma_i^m (y^i - \theta^\top x^i)^2}{2\sigma^2}\right)$$

Likelihood

$$p(\theta) \propto \exp(-\lambda \|\theta\|_1)$$

Laplacian Prior

$$p(\theta | \{x^i, y^i\}_{i=1}^m) = \frac{\prod_{i=1}^m p(y^i | x^i, \theta) p(\theta)}{\int \prod_{i=1}^m p(y^i | x^i, \theta) p(\theta) d\theta}$$

Posterior: Bayes' Rule

$$\max_{\theta} \log p(\theta | \{x^i, y^i\}_{i=1}^m) = \log L(\theta) + \log p(\theta)$$

$$\propto -\frac{1}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2 - \lambda \|\theta\|_1$$

Lasso

Select Optimizer

$$\min_{\theta} \; -\log p(\theta | \{x^i, y^i\}_{i=1}^{m}) \propto \frac{1}{m} \sum_{i=1}^{m} (y^i - \theta^\top x^i)^2 + \lambda \|\theta\|_2^2$$

- Necessary Condition
- (Stochastic) Gradient Descent

Necessary Condition

$$\min_{\theta} \; -\log p(\theta|\{x^i, y^i\}_{i=1}^m) \propto \frac{1}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)^2 + \lambda\|\theta\|_2^2$$

$$\frac{\partial \log L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}(y^i - \theta^\top x^i)x^i \qquad \frac{\partial \lambda \theta^\top \theta}{\partial \theta} = 2\lambda\theta$$

$$\frac{2}{m}\sum_{i=1}^{m} y^i x^i - \frac{2}{m}\sum_{i=1}^{m} x^i (x^i)^\top \theta + 2\lambda\theta = 0$$

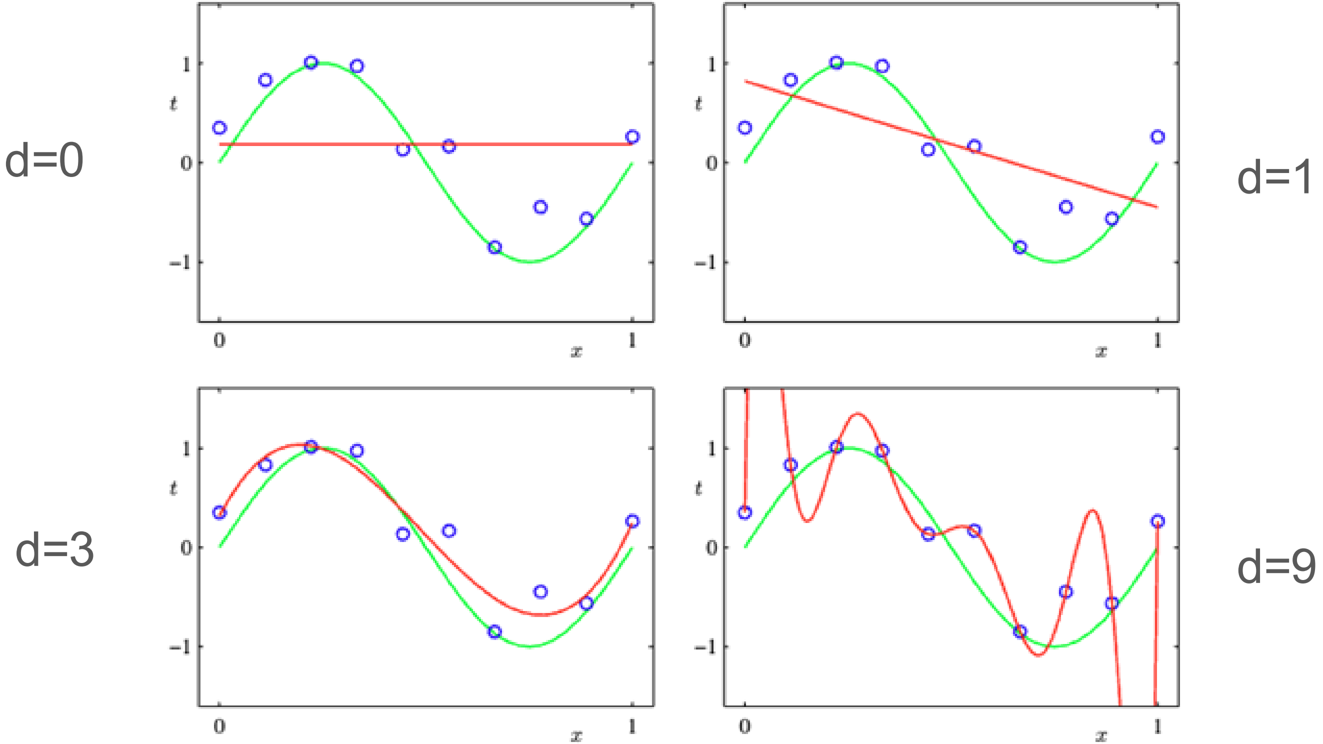
Necessary Condition

$$\frac{2}{m}\sum_{i=1}^{m} y^i x^i - \frac{2}{m}\sum_{i=1}^{m} x^i (x^i)^\top \theta + 2\lambda\theta = 0$$

$$\frac{2}{m} X y - \frac{2}{m} X X^\top \theta + 2\lambda\theta = 0$$

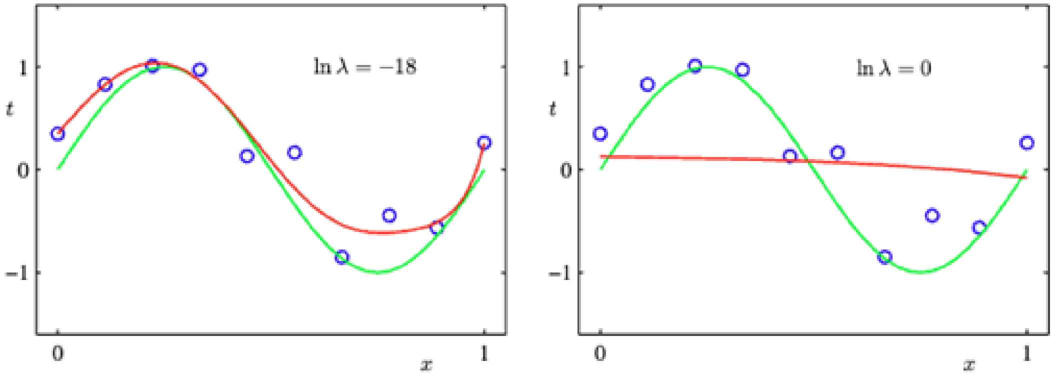
$$\Rightarrow \hat{\theta} = (X X^\top + \lambda m I)^{-1} X y$$

Overfitting with Increased Degree



Best Degree?

d=9



$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
0.35	0.35	0.13
232.37	4.74	-0.05
-5321.83	-0.77	-0.06
48568.31	-31.97	-0.05
-231639.30	-3.89	-0.03
640042.26	55.28	-0.02
-1061800.52	41.32	-0.01
1042400.18	-45.95	-0.00
-557682.99	-91.53	0.00
125201.43	72.68	0.01

- MLE with appropriate d
- MAP with large d, regularization will select the appropriate model

MLE vs. MAP

MLE

- We chose the “best” θ that maximized the likelihood given data
- No prior

$$\hat{\theta} = (XX^\top)^{-1}Xy$$

- Numerical issue
- Overfitting

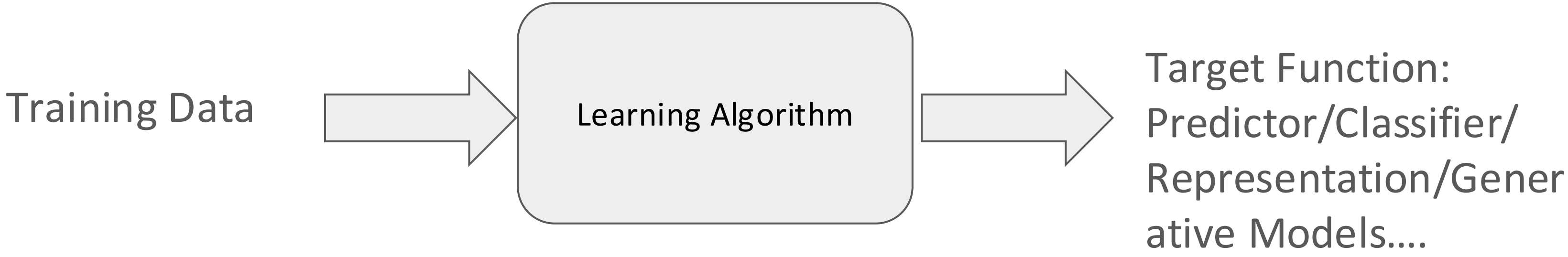
MAP

- We chose the “best” θ that maximized the posterior given data
- Prior matters

$$\hat{\theta} = (XX^\top + \lambda mI)^{-1}Xy$$

- No numerical issue
- Mitigate overfitting

ML Algorithm Pipeline



General ML Algorithm Pipeline

1. Build probabilistic models
2. Derive loss function (by MLE/MAP, maximum margin, contrastive…)
3. Select optimizer

Q&A