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Madhavan Mukund

https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning
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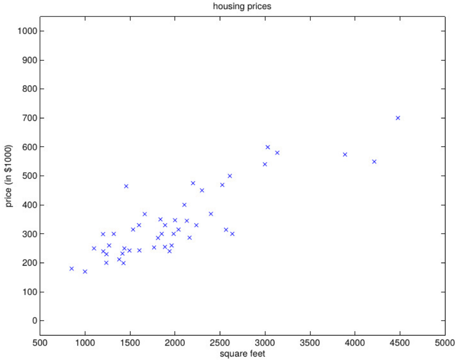
Predicting numerical values

- Data about housing prices
- Predict house price from living area

Living area (feet^2)	Price (1000\$s)
2104	400
1600	330
2400	369
1416	232
3000	540
⋮	⋮

- Scatterplot corresponding to the data
- Fit a function to the points



Linear predictors

- A richer set of input data
- Simplest case: fit a linear function with parameters $\theta = (\theta_0, \theta_1, \theta_2)$

  $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2$
- Input x may have k features $(x_1, x_2, \ldots, x_k)$
- By convention, add a dummy feature $x_0 = 1$
- For k input features

  $$h_\theta(x) = \sum_{i=0}^{k} \theta_i x_i$$

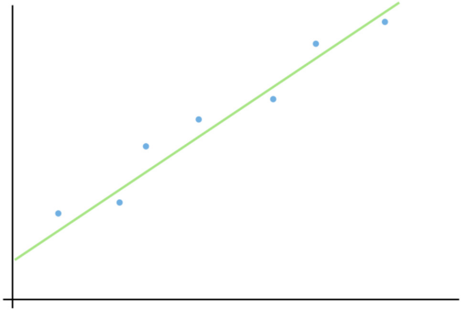
Living area (feet^2)	#bedrooms	Price (1000\$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
⋮	⋮	⋮

Finding the best fit line

- Training input is $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
  - Each input x_i is a vector $(x_i^1, \dots, x_i^k)$
  - Add $x_i^0 = 1$ by convention
  - y_i is actual output
- How far away is our prediction $h_\theta(x_i)$ from the true answer y_i?
- Define a cost (loss) function

$$J(\theta) = \frac{1}{2}\sum_{i=0}^{n}(h_\theta(x_i) - y_i)^2$$

- Essentially, the sum squared error (SSE)
- Divide by n, mean squared error (MSE)



Minimizing SSE

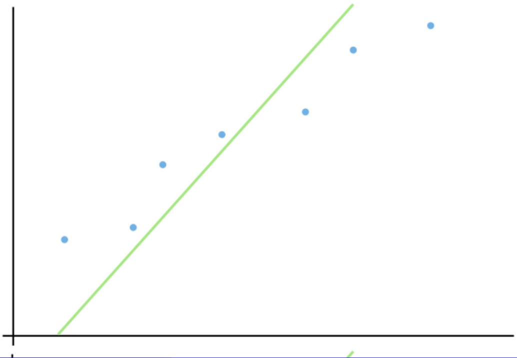
- Write x_i as row vector $\left[\begin{array}{cccc} 1 & x_i^1 & \cdots & x_i^k \end{array}\right]$
- $X = \left[\begin{array}{cccc} 1 & x_1^1 & \cdots & x_1^k \\ 1 & x_2^1 & \cdots & x_2^k \\ & & \cdots & \\ 1 & x_i^1 & \cdots & x_i^k \\ & & \cdots & \\ 1 & x_n^1 & \cdots & x_n^k \end{array}\right]$, $y = \left[\begin{array}{c} y_1 \\ y_2 \\ \cdots \\ y_i \\ \cdots \\ y_n \end{array}\right]$
- Write θ as column vector, $\theta^T = \left[\begin{array}{cccc} \theta_0 & \theta_1 & \cdots & \theta_k \end{array}\right]$
- $J(\theta) = \frac{1}{2}\sum_{i=1}^{n}(h_\theta(x_i) - y_i)^2 = \frac{1}{2}(X\theta - y)^T(X\theta - y)$
- Minimize $J(\theta)$ — set $\nabla_\theta\, J(\theta) = 0$

Minimizing SSE

- $J(\theta) = \dfrac{1}{2}(X\theta - y)^T(X\theta - y)$
- $\nabla_\theta\, J(\theta) = \nabla_\theta\, \frac{1}{2}(X\theta - y)^T(X\theta - y)$
- To minimize, set $\nabla_\theta\, \frac{1}{2}(X\theta - y)^T(X\theta - y) = 0$
- Expand, $\frac{1}{2}\nabla_\theta\, (\theta^T X^T X\theta - y^T X\theta - \theta^T X^T y + y^T y) = 0$
  - Check that $y^T X\theta = \theta^T X^T y = \displaystyle\sum_{i=1}^{n} h_\theta(x_i) \cdot y_i$
- Combining terms, $\frac{1}{2}\nabla_\theta\, (\theta^T X^T X\theta - 2\theta^T X^T y + y^T y) = 0$
- After differentiating, $X^T X\theta - X^T y = 0$
- Solve to get normal equation, $\theta = (X^T X)^{-1} X^T y$

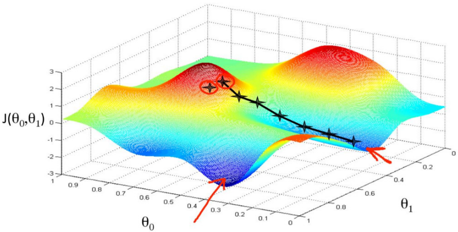
Minimizing SSE iteratively

- Normal equation $\theta = (X^T X)^{-1} X^T y$ is a closed form solution
- Computational challenges
  - Slow if n large, say $n > 10^4$
  - Matrix inversion $(X^T X)^{-1}$ is expensive, also need invertibility
- Iterative approach, make an initial guess
- Keep adjusting the line to reduce SSE
- Stop when we find the best fit line
- How do we adjust the line?



Gradient descent

- How does cost vary with parameters $\theta = (\theta_0, \theta_1, \ldots, \theta_k)$?
  - Gradients $\frac{\partial}{\partial \theta_i} J(\theta)$
- Adjust each parameter against gradient
  - $\theta_i = \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta)$



- For a single training sample (x, y)

$$
\begin{aligned}
\frac{\partial}{\partial \theta_i} J(\theta) &= \frac{\partial}{\partial \theta_i} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \frac{\partial}{\partial \theta_i} \left[\left(\sum_{j=1}^{k} \theta_j(x) \right) - y \right] \quad = (h_\theta(x) - y) \cdot x_i
\end{aligned}
$$

Gradient descent

- For a single training sample (x, y), $\dfrac{\partial}{\partial \theta_i} J(\theta) = (h_\theta(x) - y) \cdot x_i$
- Over the entire training set, $\dfrac{\partial}{\partial \theta_i} J(\theta) = \displaystyle\sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i$

Batch gradient descent

- Compute $h_\theta(x_j)$ for entire training set $\{(x_1, y_1), \ldots, (x_n, y_n)\}$
- Adjust each parameter

$$\begin{aligned}\theta_i &= \theta_i - \alpha \frac{\partial}{\partial \theta_i} J(\theta) \\ &= \theta_i - \alpha \cdot \sum_{j=1}^{n} (h_\theta(x_j) - y_j) \cdot x_j^i\end{aligned}$$

- Repeat until convergence

Stochastic gradient descent

- For each input x_j, compute $h_\theta(x_j)$
- Adjust each parameter — $\theta_i = \theta_i - \alpha \cdot (h_\theta(x_j) - y) \cdot x_j^i$

Pros and cons

- Faster progress for large batch size
- May oscillate indefinitely

Regression and SSE loss

- Training input is $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$
  - Noisy outputs from a linear function
  - $y_i = \theta^T x_i + \epsilon$
  - $\epsilon \sim \mathcal{N}(0, \sigma^2)$: Gaussian noise, mean 0, fixed variance σ^2
  - $y_i \sim \mathcal{N}(\mu_i, \sigma^2)$, $\mu_i = \theta^T x_i$
- Model gives us an estimate for θ, so regression learns μ_i for each x_i
- Want Maximum Likelihood Estimator (MLE) — maximize
  $$\mathcal{L}(\theta) = \prod_{i=1}^{n} P(y_i \mid x_i; \theta)$$
- Instead, maximize log likelihood
  $$\ell(\theta) = \log \left(\prod_{i=1}^{n} P(y_i \mid x_i; \theta) \right) = \sum_{i=1}^{n} \log(P(y_i \mid x_i; \theta))$$

Log likelihood and SSE loss

- $y_i = \mathcal{N}(\mu_i, \sigma^2)$, so $P(y_i \mid x_i; \theta) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu_i)^2}{2\sigma^2}} = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\theta^T x_i)^2}{2\sigma^2}}$

- Log likelihood (assuming natural logarithm)

$$\ell(\theta) = \sum_{i=1}^{n} \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\theta^T x_i)^2}{2\sigma^2}}\right) = n \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) - \sum_{i=1}^{n} \frac{(y-\theta^T x_i)^2}{2\sigma^2}$$

- To maximize $\ell(\theta)$ with respect to θ, ignore all terms that do not depend on θ

- Optimum value of θ is given by

$$\hat{\theta}_{\text{MSE}} = \arg\max_{\theta} \left[-\sum_{i=1}^{n} (y_i - \theta^T x_i)^2\right] = \arg\min_{\theta} \left[\sum_{i=1}^{n} (y_i - \theta^T x_i)^2\right]$$

- Assuming data points are generated by linear function and then perturbed by Gaussian noise, SSE is the “correct” loss function to maximize likelihood