

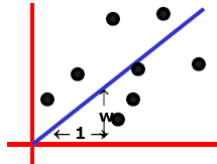
Machine Learning

10-701/15-781, Fall 2012

Linear Regression and Sparsity

Eric Xing

Lecture 5, September 24, 2012



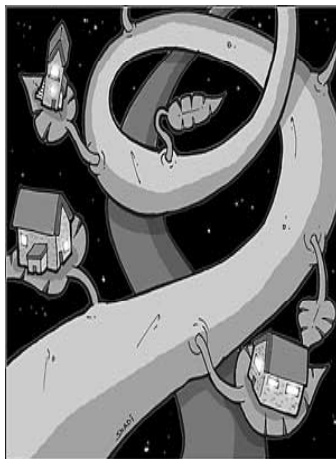
Reading:

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Machine learning for apartment hunting



- Now you've moved to Pittsburgh!!
And you want to find the **most reasonably priced** apartment satisfying your **needs**:



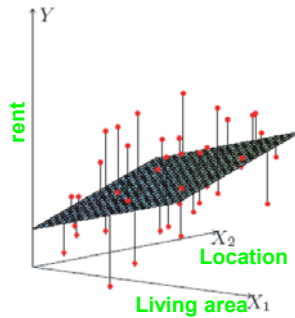
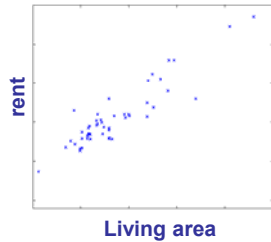
square-ft., # of bedroom, distance to campus ...

Living area (ft ²)	# bedroom	Rent (\$)
230	1	600
506	2	1000
433	2	1100
109	1	500
...		
150	1	?
270	1.5	?

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The learning problem

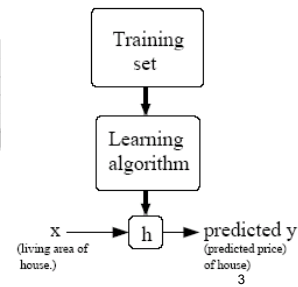


- Features:
 - Living area, distance to campus, # bedroom ...
 - Denote as $\mathbf{x}=[x^1, x^2, \dots, x^k]$
- Target:
 - Rent
 - Denoted as y
- Training set:

Our goal:

$$\mathbf{X} = \begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \mathbf{x}_2 & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{x}_n & - \end{bmatrix} = \begin{bmatrix} x_1^1 & x_1^2 & \dots & x_1^k \\ x_2^1 & x_2^2 & \dots & x_2^k \\ \vdots & \vdots & \vdots & \vdots \\ x_n^1 & x_n^2 & \dots & x_n^k \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} - & y_1 & - \\ - & y_2 & - \\ \vdots & \vdots & \vdots \\ - & y_n & - \end{bmatrix}$$



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Linear Regression



- Assume that Y (target) is a linear function of X (features):
 - e.g.:

$$\hat{y} = \theta_0 + \theta_1 x^1 + \theta_2 x^2$$
 - let's assume a vacuous "feature" $x^0=1$ (this is the **intercept term**, why?), and define the feature vector to be:
 - then we have the following general representation of the linear function:
- Our goal is to pick the optimal θ . How!
 - We seek θ that minimize the following **cost function**:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^n (\hat{y}_i(\bar{x}_i) - y_i)^2$$

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The Least-Mean-Square (LMS) method



- The Cost Function:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i^T \theta - y_i)^2$$

- Consider a **gradient descent** algorithm:

$$\theta_j^{t+1} = \theta_j^t - \alpha \left. \frac{\partial}{\partial \theta_j} J(\theta) \right|_t$$

The Least-Mean-Square (LMS) method



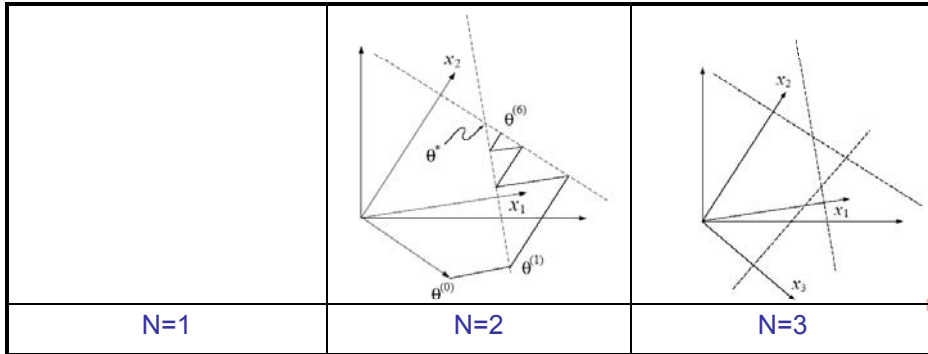
- Now we have the following descent rule:

$$\theta_j^{t+1} = \theta_j^t + \alpha \sum_{i=1}^n (y_i - \bar{\mathbf{x}}_i^T \theta^t) x_i^j$$

- For a single training point, we have:

- This is known as the LMS update rule, or the Widrow-Hoff learning rule
- This is actually a "**stochastic**", "**coordinate**" descent algorithm
- This can be used as a **on-line** algorithm

Geometric and Convergence of LMS



$$\theta^{t+1} = \theta^t + \alpha(y_i - \bar{\mathbf{x}}_i^T \theta^t) \bar{\mathbf{x}}_i$$

Claim: when the step size α satisfies certain condition, and when certain other technical conditions are satisfied, LMS will converge to an “optimal region”.

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Steepest Descent and LMS

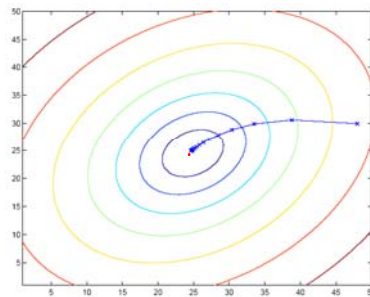


- Steepest descent

- Note that:

$$\nabla_{\theta} J = \left[\frac{\partial}{\partial \theta_1} J, \dots, \frac{\partial}{\partial \theta_k} J \right]^T = - \sum_{i=1}^n (y_n - \mathbf{x}_n^T \theta) \mathbf{x}_n$$

$$\theta^{t+1} = \theta^t + \alpha \sum_{i=1}^n (y_n - \mathbf{x}_n^T \theta^t) \mathbf{x}_n$$



- This is as a **batch** gradient descent algorithm

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The normal equations



- Write the cost function in matrix form:

$$\begin{aligned} J(\theta) &= \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i^T \theta - y_i)^2 \\ &= \frac{1}{2} (X\theta - \bar{y})^T (X\theta - \bar{y}) \\ &= \frac{1}{2} (\theta^T X^T X \theta - \theta^T X^T \bar{y} - \bar{y}^T X \theta + \bar{y}^T \bar{y}) \end{aligned}$$

$$\mathbf{X} = \begin{bmatrix} \text{---} & \mathbf{x}_1 & \text{---} \\ \text{---} & \mathbf{x}_2 & \text{---} \\ \vdots & \vdots & \vdots \\ \text{---} & \mathbf{x}_n & \text{---} \end{bmatrix}$$

$$\bar{\mathbf{y}} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- To minimize $J(\theta)$, take derivative and set to zero:

$$\begin{aligned} \nabla_{\theta} J &= \frac{1}{2} \nabla_{\theta} \text{tr}(\theta^T X^T X \theta - \theta^T X^T \bar{y} - \bar{y}^T X \theta + \bar{y}^T \bar{y}) \\ &= \frac{1}{2} (\nabla_{\theta} \text{tr} \theta^T X^T X \theta - 2 \nabla_{\theta} \text{tr} \bar{y}^T X \theta + \nabla_{\theta} \text{tr} \bar{y}^T \bar{y}) \\ &= \frac{1}{2} (X^T X \theta + X^T X \theta - 2 X^T \bar{y}) \\ &= X^T X \theta - X^T \bar{y} = 0 \end{aligned}$$

$$\Rightarrow \boxed{X^T X \theta = X^T \bar{y}}$$

The normal equations

$$\Downarrow$$

$$\theta^* = (X^T X)^{-1} X^T \bar{y}$$

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Some matrix derivatives



- For $f: \mathbb{R}^{m \times n} \mapsto \mathbb{R}$, define:

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial}{\partial A_{11}} f & \cdots & \frac{\partial}{\partial A_{1n}} f \\ \vdots & \ddots & \vdots \\ \frac{\partial}{\partial A_{1m}} f & \cdots & \frac{\partial}{\partial A_{mn}} f \end{bmatrix}$$

- Trace:

$$\text{tr} A = \sum_{i=1}^n A_{ii}, \quad \text{tr} a = a, \quad \text{tr} ABC = \text{tr} CAB = \text{tr} BCA$$

- Some fact of matrix derivatives (without proof)

$$\nabla_A \text{tr} AB = B^T, \quad \nabla_A \text{tr} ABA^T C = CAB + C^T AB^T, \quad \nabla_A |A| = |A| (A^{-1})^T$$

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Comments on the normal equation



- In most situations of practical interest, the number of data points N is larger than the dimensionality k of the input space and the matrix \mathbf{X} is of full column rank. If this condition holds, then it is easy to verify that $X^T X$ is necessarily invertible.
- The assumption that $X^T X$ is invertible implies that it is positive definite, thus at the critical point we have found is a minimum.
- What if \mathbf{X} has less than full column rank? \rightarrow regularization (later).

Direct and Iterative methods



- Direct methods: we can achieve the solution in a single step by solving the normal equation
 - Using Gaussian elimination or QR decomposition, we converge in a finite number of steps
 - It can be infeasible when data are streaming in in real time, or of very large amount
- Iterative methods: stochastic or steepest gradient
 - Converging in a limiting sense
 - But more attractive in large practical problems
 - Caution is needed for deciding the learning rate α



Convergence rate

- **Theorem:** the steepest descent equation algorithm converge to the minimum of the cost characterized by normal equation:

$$\theta^{(\infty)} = (X^T X)^{-1} X^T y$$

If

$$0 < \alpha < 2/\lambda_{\max}[X^T X]$$

- A formal analysis of LMS need more math-mussels; in practice, one can use a small α , or gradually decrease α .



A Summary:

- LMS update rule

$$\theta_j^{t+1} = \theta_j^t + \alpha(y_n - \mathbf{x}_n^T \theta^t) \mathbf{x}_{n,i}$$

- Pros: on-line, low per-step cost, fast convergence and perhaps less prone to local optimum
- Cons: convergence to optimum not always guaranteed

- Steepest descent

$$\theta^{t+1} = \theta^t + \alpha \sum_{i=1}^n (y_n - \mathbf{x}_n^T \theta^t) \mathbf{x}_n$$

- Pros: easy to implement, conceptually clean, guaranteed convergence
- Cons: batch, often slow converging

- Normal equations

$$\theta^* = (X^T X)^{-1} X^T \bar{y}$$

- Pros: a single-shot algorithm! Easiest to implement.
- Cons: need to compute pseudo-inverse $(X^T X)^{-1}$, expensive, numerical issues (e.g., matrix is singular ..), although there are ways to get around this ...

Geometric Interpretation of LMS



- The predictions on the training data are:

$$\hat{\mathbf{y}} = X\theta^* = X(X^T X)^{-1} X^T \bar{\mathbf{y}}$$

- Note that

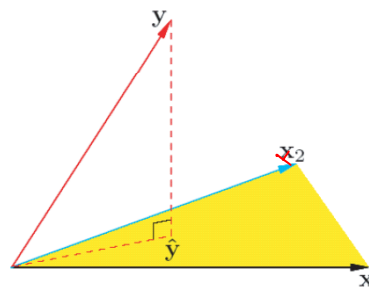
$$\hat{\mathbf{y}} - \bar{\mathbf{y}} = (X(X^T X)^{-1} X^T - I)\bar{\mathbf{y}}$$

and

$$\begin{aligned} X^T(\hat{\mathbf{y}} - \bar{\mathbf{y}}) &= X^T(X(X^T X)^{-1} X^T - I)\bar{\mathbf{y}} \\ &= (X^T X(X^T X)^{-1} X^T - X^T)\bar{\mathbf{y}} \\ &= \mathbf{0} \quad !! \end{aligned}$$

$\hat{\mathbf{y}}$ is the orthogonal projection of $\bar{\mathbf{y}}$ into the space spanned by the column of X

$$\bar{\mathbf{y}} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} - & \mathbf{x}_1 & - \\ - & \mathbf{x}_2 & - \\ \vdots & \vdots & \vdots \\ - & \mathbf{x}_n & - \end{bmatrix}$$



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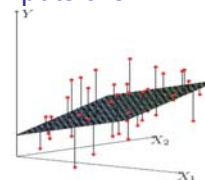
Probabilistic Interpretation of LMS



- Let us assume that the target variable and the inputs are related by the equation:

$$y_i = \theta^T \mathbf{x}_i + \varepsilon_i$$

where ε is an error term of unmodeled effects or random noise



- Now assume that ε follows a Gaussian $\mathcal{N}(0, \sigma)$, then we have:

$$p(y_i | x_i; \theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

- By independence assumption:

$$L(\theta) = \prod_{i=1}^n p(y_i | x_i; \theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n \exp\left(-\frac{\sum_{i=1}^n (y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

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Probabilistic Interpretation of LMS, cont.



- Hence the log-likelihood is:

$$l(\theta) = n \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \frac{1}{2} \sum_{i=1}^n (y_i - \theta^T \mathbf{x}_i)^2$$

- Do you recognize the last term?

Yes it is: $J(\theta) = \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i^T \theta - y_i)^2$

- Thus under independence assumption, LMS is equivalent to MLE of θ !

Case study: predicting gene expression



The genetic picture

causal SNPs

CGTTTCACTGTACAATTT



a univariate phenotype:

i.e., the expression intensity of a gene

Association Mapping as Regression



	Phenotype (BMI)	Genotype
Individual 1	2.5	C T C T
		C A C T
Individual 2	4.8	G A G A
		C T C T
⋮		
Individual N	4.7	G T C T
		G T G T

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Association Mapping as Regression



	Phenotype (BMI)	Genotype
Individual 1	2.5	.. 0 1 . . 0 0
Individual 2	4.8	.. 1 1 . . 1 1
⋮		
Individual N	4.7	.. 2 2 . . 1 0

$y_i = \sum_{j=1}^J x_{ij} \beta_j$

SNPs with large $|\beta_j|$ are relevant

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Experimental setup

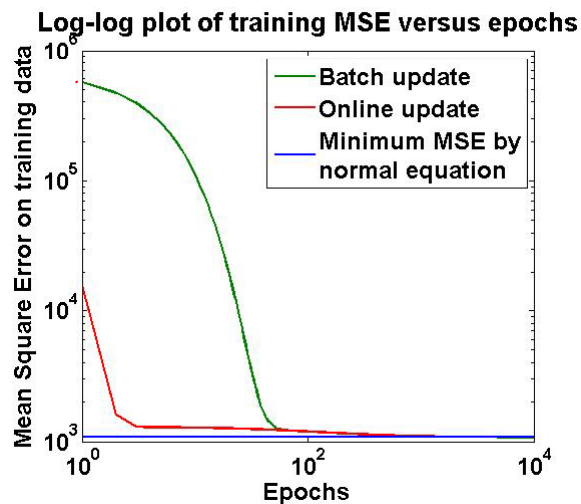


- Asthama dataset
 - 543 individuals, genotyped at 34 SNPs
 - Diploid data was transformed into 0/1 (for homozygotes) or 2 (for heterozygotes)
 - $X=543 \times 34$ matrix
 - Y =Phenotype variable (continuous)
- A single phenotype was used for regression
- Implementation details
 - Iterative methods: Batch update and online update implemented.
 - For both methods, step size α is chosen to be a small fixed value (10^{-6}). This choice is based on the data used for experiments.
 - Both methods are only run to a maximum of 2000 epochs or until the change in training MSE is less than 10^{-4}

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Convergence Curves

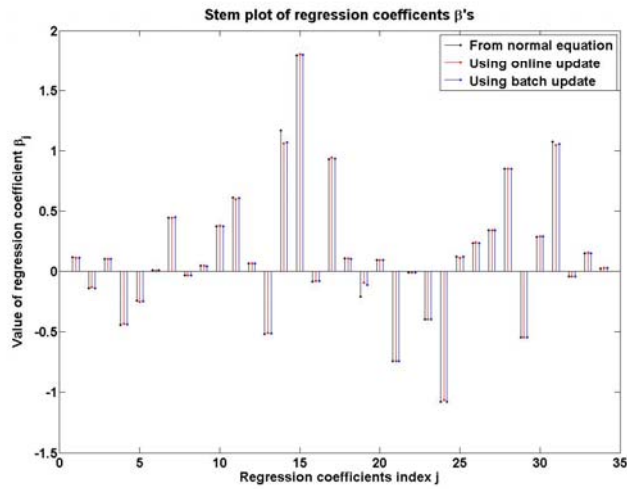


- For the batch method, the training MSE is initially large due to uninformed initialization
- In the online update, N updates for every epoch reduces MSE to a much smaller value.

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The Learned Coefficients



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Multivariate Regression for Trait Association Analysis



Trait Genotype Association Strength

2.1 = TGAACCATGAAGTA x ?

$$y = Xx\beta$$

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Multivariate Regression for Trait Association Analysis



Trait Genotype Association Strength

2.1

=

T
G
A
A
C
C
A
T
G
A
A
G
T
A

X



$$\beta^* = \arg \min_{\beta} (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$

Many non-zero associations:
Which SNPs are truly significant?

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Sparsity



- One common assumption to make **sparsity**.
- **Makes biological sense**: each phenotype is likely to be associated with a small number of SNPs, rather than all the SNPs.
- **Makes statistical sense**: Learning is now feasible in high dimensions with small sample size

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Sparsity: In a mathematical sense

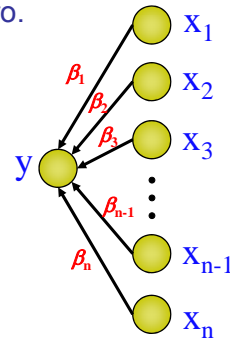


- Consider least squares linear regression problem:
- Sparsity means most of the beta's are zero.

$$\hat{\beta} = \operatorname{argmin}_{\beta} \|\mathbf{Y} - \mathbf{X}\beta\|^2$$

subject to:

$$\sum_{j=1}^p \mathbb{I}[|\beta_j| > 0] \leq C$$



- But this is not convex!!! Many local optima, computationally intractable.

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L1 Regularization (LASSO)

(Tibshirani, 1996)



- A convex relaxation.

Constrained Form

$$\hat{\beta} = \operatorname{argmin}_{\beta} \|\mathbf{Y} - \mathbf{X}\beta\|^2$$

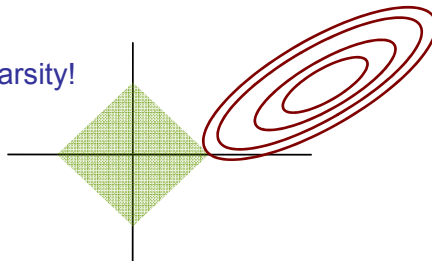
subject to:

$$\sum_{j=1}^p |\beta_j| \leq C$$

Lagrangian Form

$$\hat{\beta} = \operatorname{argmin}_{\beta} \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_1$$

- Still enforces sparsity!



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Bayesian Interpretation



- Treat the distribution parameters θ also as a *random variable*
- The *a posteriori* distribution of θ after seen the data is:

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} = \frac{p(D|\theta)p(\theta)}{\int p(D|\theta)p(\theta)d\theta}$$

This is Bayes Rule

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}$$

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London*, 53:370-418



The prior $p(\cdot)$ encodes our prior knowledge about the domain

Regularized Least Squares and MAP



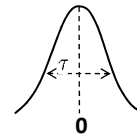
What if $(X^T X)$ is not invertible ?

$$\hat{\beta}_{\text{MAP}} = \arg \max_{\beta} \underbrace{\log p(\{(X_i, Y_i)\}_{i=1}^n | \beta, \sigma^2)}_{\text{log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

1) Gaussian Prior

$$\beta \sim \mathcal{N}(0, \tau^2 \mathbf{I})$$

$$p(\beta) \propto e^{-\beta^T \beta / 2\tau^2}$$



$$\hat{\beta}_{\text{MAP}} = \arg \min_{\beta} \sum_{i=1}^n (Y_i - X_i \beta)^2 + \lambda \|\beta\|_2^2$$

Ridge Regression

Closed form: HW

constant(σ^2, τ^2)

Prior belief that β is Gaussian with zero-mean biases solution to "small" β

Regularized Least Squares and MAP



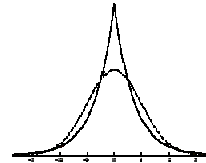
What if $(X^T X)$ is not invertible ?

$$\hat{\beta}_{\text{MAP}} = \arg \max_{\beta} \underbrace{\log p(\{(X_i, Y_i)\}_{i=1}^n | \beta, \sigma^2)}_{\text{log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

II) Laplace Prior

$\beta_i \stackrel{iid}{\sim} \text{Laplace}(0, t)$

$$p(\beta_i) \propto e^{-|\beta_i|/t}$$



$$\hat{\beta}_{\text{MAP}} = \arg \min_{\beta} \sum_{i=1}^n (Y_i - X_i \beta)^2 + \lambda \|\beta\|_1 \quad \text{Lasso}$$

\downarrow
 constant(σ^2, t)

Prior belief that β is Laplace with zero-mean biases solution to "small" β

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Take home message



- Gradient descent
 - On-line
 - Batch
- Normal equations
- Geometric interpretation of LMS
- Probabilistic interpretation of LMS, and equivalence of LMS and MLE under certain assumption (what?)
- Sparsity:
 - Approach: ridge vs. lasso regression
 - Interpretation: regularized regression versus Bayesian regression
 - Algorithm: convex optimization (we did not discuss this)
- LR does not mean fitting linear relations, but linear combination or basis functions (that can be non-linear)
- Weighting points by importance versus by fitness

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Advanced Material: Beyond basic LR



- LR with non-linear basis functions
- Locally weighted linear regression
- Regression trees and Multilinear Interpolation

**We will discuss this in next class after we set the state right!
(if we've got time 😊)**

Non-linear functions:



LR with non-linear basis functions



- LR does not mean we can only deal with linear relationships
- We are free to design (non-linear) features under LR

$$y = \theta_0 + \sum_{j=1}^m \theta_j \phi_j(x) = \theta^T \phi(x)$$

where the $\phi_j(x)$ are fixed basis functions (and we define $\phi_0(x) = 1$).

- Example: polynomial regression:

$$\phi(x) := [1, x, x^2, x^3]$$

- We will be concerned with estimating (distributions over) the weights θ and choosing the model order M .

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Basis functions



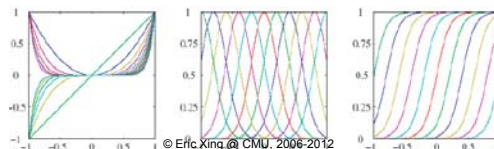
- There are many basis functions, e.g.:

- Polynomial $\phi_j(x) = x^{j-1}$

- Radial basis functions $\phi_j(x) = \exp\left(-\frac{(x - \mu_j)^2}{2s^2}\right)$

- Sigmoidal $\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$

- Splines, Fourier, Wavelets, etc



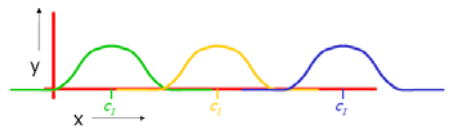
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1D and 2D RBFs

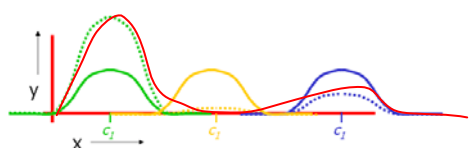


- 1D RBF



$$y^{est} = \beta_1 \phi_1(x) + \beta_2 \phi_2(x) + \beta_3 \phi_3(x)$$

- After fit:



$$y^{est} = 2\phi_1(x) + 0.05\phi_2(x) + 0.5\phi_3(x)$$

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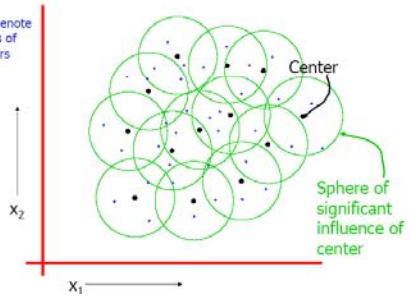
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Good and Bad RBFs

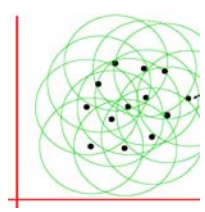
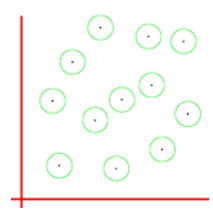


- A good 2D RBF

Blue dots denote coordinates of input vectors



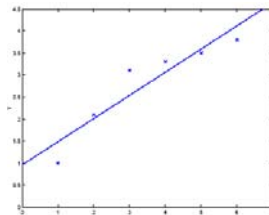
- Two bad 2D RBFs



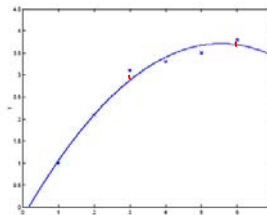
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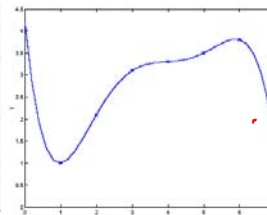
Overfitting and underfitting



$$y = \theta_0 + \theta_1 x$$



$$y = \theta_0 + \theta_1 x + \theta_2 x^2$$



$$y = \sum_{j=0}^5 \theta_j x^j$$

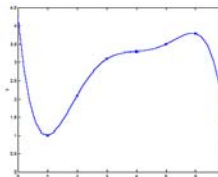
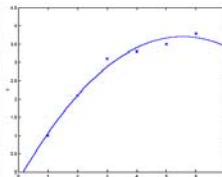
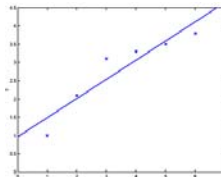
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Bias and variance



- We define the bias of a model to be the expected generalization error even if we were to fit it to a very (say, infinitely) large training set.
- By fitting "spurious" patterns in the training set, we might again obtain a model with large generalization error. In this case, we say the model has large variance.



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Locally weighted linear regression

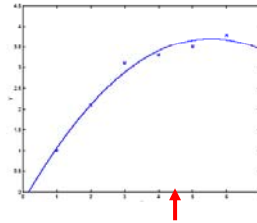


- The algorithm:

Instead of minimizing $J(\theta) = \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i^T \theta - y_i)^2$

now we fit θ to minimize $J(\theta) = \frac{1}{2} \sum_{i=1}^n w_i (\mathbf{x}_i^T \theta - y_i)^2$

Where do w_i 's come from? $w_i = \exp\left(-\frac{(\mathbf{x}_i - \mathbf{x})^2}{2\tau^2}\right)$



- where \mathbf{x} is the query point for which we'd like to know its corresponding y

→ Essentially we put higher weights on (errors on) training examples that are close to the query point (than those that are further away from the query)

Parametric vs. non-parametric

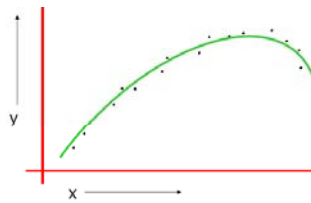
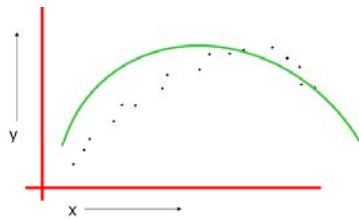


- Locally weighted linear regression is the second example we are running into of a **non-parametric** algorithm. (what is the first?)
- The (unweighted) linear regression algorithm that we saw earlier is known as a **parametric** learning algorithm
 - because it has a fixed, finite number of parameters (the θ), which are fit to the data;
 - Once we've fit the θ and stored them away, we no longer need to keep the training data around to make future predictions.
 - In contrast, to make predictions using locally weighted linear regression, we need to keep the entire training set around.
- The term "**non-parametric**" (roughly) refers to the fact that the amount of stuff we need to keep in order to represent the hypothesis grows linearly with the size of the training set.

Robust Regression



- The best fit from a quadratic regression
- But this is probably better ...



How can we do this?

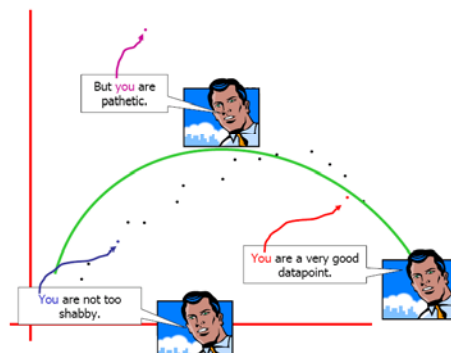
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LOESS-based Robust Regression



- Remember what we do in "locally weighted linear regression"?
→ we "score" each point for its impotence
- Now we score each point according to its "fitness"



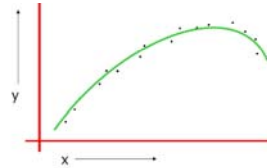
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(Courtesy to Andrgw Moor)

Robust regression



- For $k = 1$ to $R \dots$
 - Let (x_k, y_k) be the k th datapoint
 - Let y_k^{est} be predicted value of y_k
 - Let w_k be a weight for data point k that is large if the data point fits well and small if it fits badly:



$$w_k = \phi((y_k - y_k^{\text{est}})^2)$$

- Then redo the regression using weighted data points.
- Repeat whole thing until converged!

Robust regression—probabilistic interpretation



- What regular regression does:

Assume y_k was originally generated using the following recipe:

$$y_k = \theta^T \mathbf{x}_k + \mathcal{N}(0, \sigma^2)$$

Computational task is to find the Maximum Likelihood estimation of θ

Robust regression—probabilistic interpretation



- What LOESS robust regression does:

Assume y_k was originally generated using the following recipe:

with probability p : $y_k = \theta^T \mathbf{x}_k + \mathcal{N}(0, \sigma^2)$

but otherwise $y_k \sim \mathcal{N}(\mu, \sigma_{\text{huge}}^2)$

Computational task is to find the Maximum Likelihood estimates of θ , p , μ and σ_{huge} .

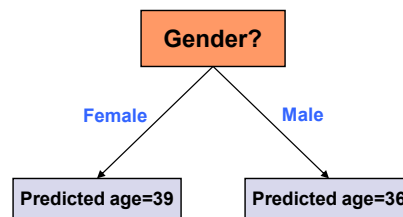
- The algorithm you saw with iterative **reweighting/refitting** does this computation for us. Later you will find that it is an instance of the famous **E.M.** algorithm

Regression Tree



- Decision tree for regression

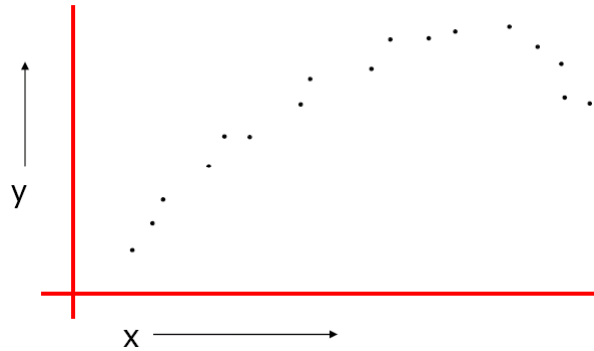
Gender	Rich?	Num. Children	# travel per yr.	Age
F	No	2	5	38
M	No	0	2	25
M	Yes	1	0	72
:	:	:	:	:



A conceptual picture



- Assuming regular regression trees, can you sketch a graph of the fitted function $y^*(x)$ over this diagram?



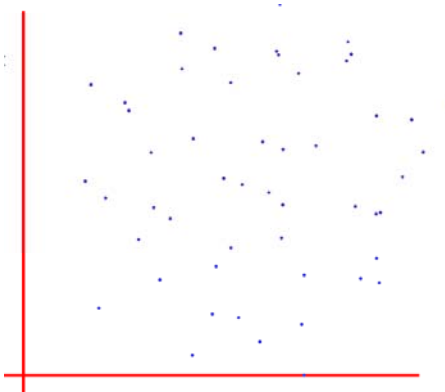
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How about this one?



- Multilinear Interpolation



- We wanted to create a continuous and piecewise linear fit to the data

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Take home message



- Gradient descent
 - On-line
 - Batch
- Normal equations
- Geometric interpretation of LMS
- Probabilistic interpretation of LMS, and equivalence of LMS and MLE under certain assumption (what?)
- Sparsity:
 - Approach: ridge vs. lasso regression
 - Interpretation: regularized regression versus Bayesian regression
 - Algorithm: convex optimization (we did not discuss this)
- LR does not mean fitting linear relations, but linear combination or basis functions (that can be non-linear)
- Weighting points by importance versus by fitness