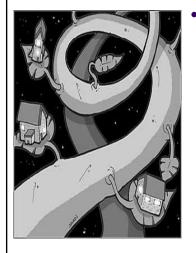


Machine learning for apartment hunting





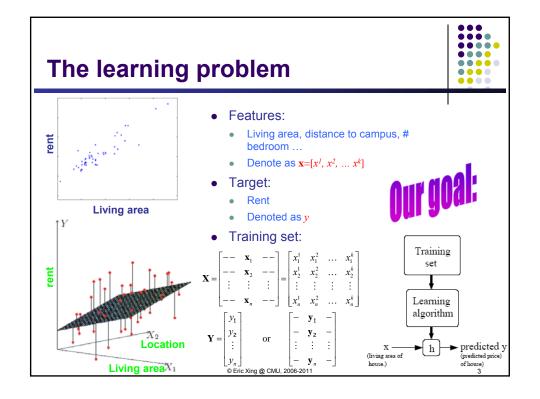
Now you've moved to Pittsburgh!!

And you want to find the **most reasonably priced** apartment satisfying your **needs**:

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

Living area (ft²)	# bedroom	Rent (\$)
230	1	600
506	2	1000
433	2	1100
109	1	500
150	1	?
270	1.5	?

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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" X⁰=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 heta that minimize the following **cost function**:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{n} (\hat{y}_{i}(\vec{x}_{i}) - y_{i})^{2}$$

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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:

$$\theta_j^{t+1} = \theta_j^t - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \bigg|_{t}$$

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The Least-Mean-Square (LMS) method



• Now we have the following descent rule:

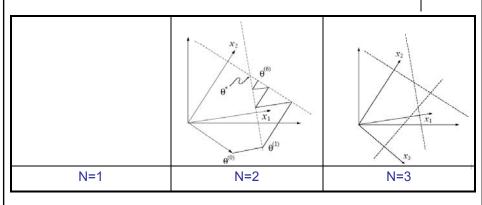
$$\theta_j^{t+1} = \theta_j^t + \alpha \sum_{i=1}^n (y_i - \bar{\mathbf{x}}_i^T \theta^t) x_i^j$$

- 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

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Geometric and Convergence of LMS





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

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

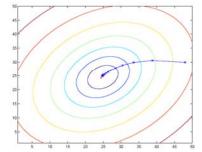
Steepest Descent and LMS



- Steepest descent
 - Note that:

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:

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

$$= \frac{1}{2} (X\theta - \vec{y})^{T} (X\theta - \vec{y})$$

$$= \frac{1}{2} (\theta^{T} X^{T} X \theta - \theta^{T} X^{T} \vec{y} - \vec{y}^{T} X \theta + \vec{y}^{T} \vec{y})$$

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

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

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

$$\nabla_{\theta} J = \frac{1}{2} \nabla_{\theta} \operatorname{tr} \left(\theta^{T} X^{T} X \theta - \theta^{T} X^{T} \bar{y} - \bar{y}^{T} X \theta + \bar{y}^{T} \bar{y} \right)$$

$$= \frac{1}{2} \left(\nabla_{\theta} \operatorname{tr} \theta^{T} X^{T} X \theta - 2 \nabla_{\theta} \operatorname{tr} \bar{y}^{T} X \theta + \nabla_{\theta} \operatorname{tr} \bar{y}^{T} \bar{y} \right)$$

$$= \frac{1}{2} \left(X^{T} X \theta + X^{T} X \theta - 2 X^{T} \bar{y} \right)$$

$$= X^{T} X \theta - X^{T} \bar{y} = \mathbf{0}$$

$$\Rightarrow X^T X \theta = X^T \vec{y}$$
The normal equations

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

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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:

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

• Some fact of matrix derivatives (without proof)

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

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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 X is of full column rank. If this condition holds, then it is easy to verify that X^TX is necessarily invertible.
- The assumption that X^TX is invertible implies that it is positive definite, thus the critical point we have found is a minimum.
- What if X has less than full column rank? → regularization (later).

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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
 - \bullet $\;$ Caution is needed for deciding the learning rate α

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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 .

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A Summary:



LMS update rule

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

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

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

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

Normal equations
$$\theta^* = (X^T X)^{-1} X^T \vec{y}$$

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

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Geometric Interpretation of LMS



• The predictions on the training data are:

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

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

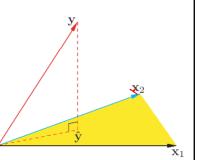
• Note that
$$\hat{\vec{y}} - \vec{y} = \left(X (X^T X)^{-1} X^T - I \right) \vec{y}$$

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

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

$$= 0 \quad !!$$

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



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Probabilistic Interpretation of LMS



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

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

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

• Now assume that ε follows a Gaussian $N(0,\sigma)$, then we have:

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

• By independence assumption:

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

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!

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Case study: predicting gene expression



The genetic picture

causal SNPs



a univariate phenotype:

i.e., the expression intensity of a gene

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\ssociat	ion Mapping	as Regression	
	Phenotype (BMI)	Genotype	
Individual 1	2.5		
Individual 2 :	4.8	GA <mark>G</mark> / CT <mark>C</mark> T	
Individual N	4.7	GT <mark>C</mark> T	
		Benign SNPs Causal	SNP
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Association Mapping as Regression			
	Phenotype (BMI)	Genotype	<u> </u>
Individual 1	2.5	0100	
Individual 2	4.8	1111	
Individual N	4.7	2210	
	•	$_J$ $lacksquare$	
	$\mathbf{y}_i =$	$\sum_{j=1}^{\sigma} x_{ij} oldsymbol{eta}_j rac{SNPs}{ oldsymbol{eta}_j }$ ar	with large e relevant
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Experimental setup



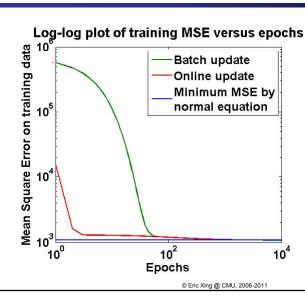
- Asthama dataset
 - 543 individuals, genotyped at 34 SNPs
 - Diploid data was transformed into 0/1 (for homozygotes) or 2 (for heterozygotes)
 - X=543x34 matrix
 - Y=Phenotype variable (continuous)
- A single phenotype was used for regression
- Implementation details
 - Iterative methods: Batch update 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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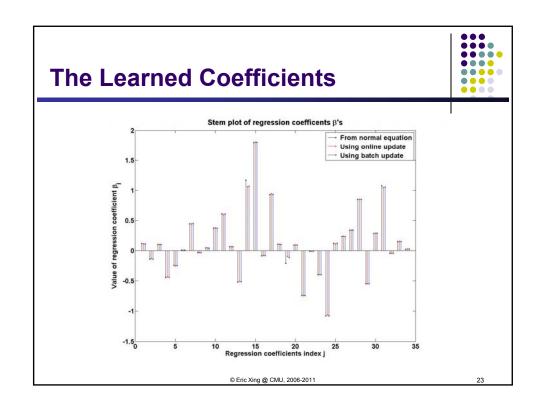
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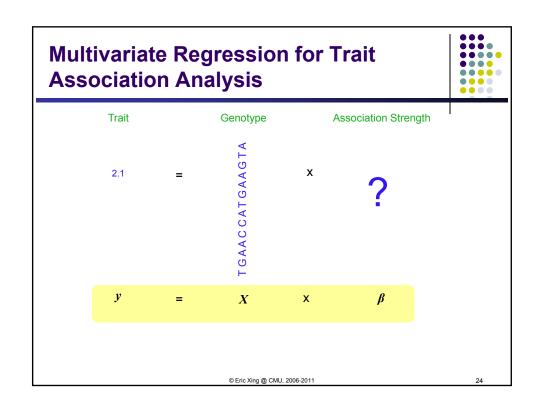
Convergence Curves

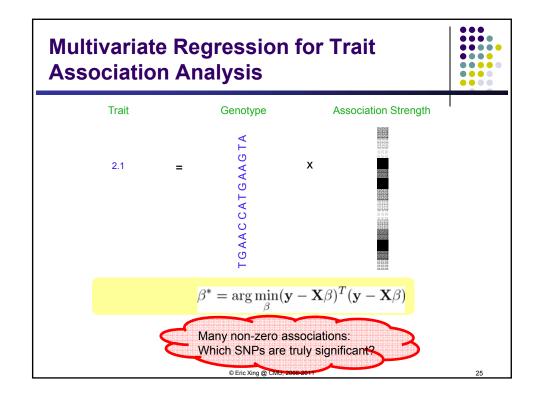




- For the batch method, the training MSE is initially large due to uninformed initialization
- In the online update, N updates for every epoch reduces MSE to a much smaller value.







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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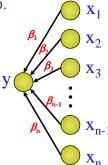
Sparsity: In a mathematical sense



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

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

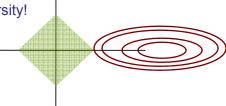
• A convex relaxation.

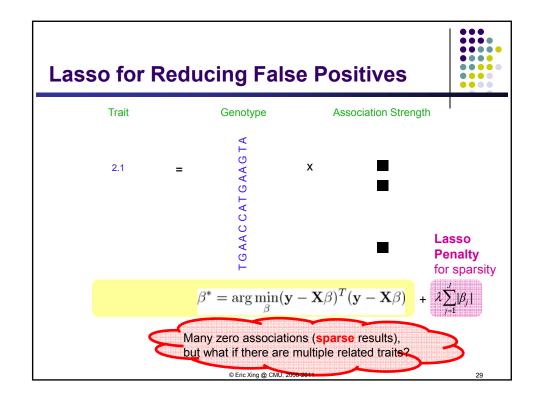
$$\hat{\boldsymbol{\beta}} = \operatorname{argmin}_{\boldsymbol{\beta}} \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|^2$$
 subject to:

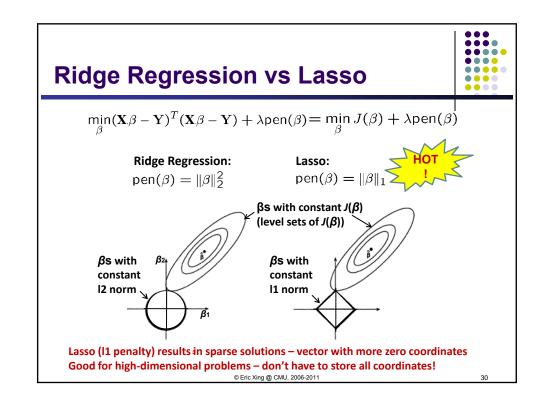
$$\hat{oldsymbol{eta}} = \mathop{\mathrm{argmin}}_{oldsymbol{eta}} \|\mathbf{Y} - \mathbf{X}oldsymbol{eta}\|^2 + \lambda \|oldsymbol{eta}\|_1$$

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

• Still enforces sparsity!







Bayesian Interpretation



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

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

This is Bayes Rule

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

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(.) encodes our prior knowledge about the domain

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Regularized Least Squares and MAP



What if (XTX) is not invertible?

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

I) Gaussian Prior

ussian Prior
$$eta \sim \mathcal{N}(\mathsf{0}, au^2 \mathrm{I})$$
 $p(eta) \propto e^{-eta^T eta/2 au^2}$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i \beta)^2 + \lambda \|\beta\|_2^2 \qquad \text{Ridge Regression}$$
 Closed form: HW

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

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Regularized Least Squares and MAP



What if (X^TX) is not invertible?

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

II) Laplace Prior

$$eta_i \stackrel{iid}{\sim} \mathsf{Laplace}(0,t) \qquad \qquad p(eta_i) \propto e^{-|eta_i|/t}$$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i \beta)^2 + \lambda \|\beta\|_1 \qquad \text{Lasso}$$
 Closed form: HW
$$\qquad \qquad \text{constant}(\sigma^2, t)$$

Prior belief that β is Laplace with zero-mean biases solution to "small" β © Eric Xing @ CMU, 2006-2011

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Beyond basic LR



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

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Non-linear functions:



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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

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

where the $\phi_l(x)$ 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



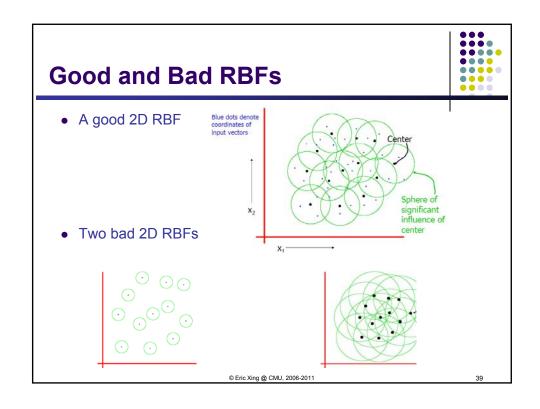
 $y^{est} = \beta_1 \phi_1(x) + \frac{\beta_2 \phi_2(x)}{\beta_3 \phi_3(x)} + \beta_3 \phi_3(x)$

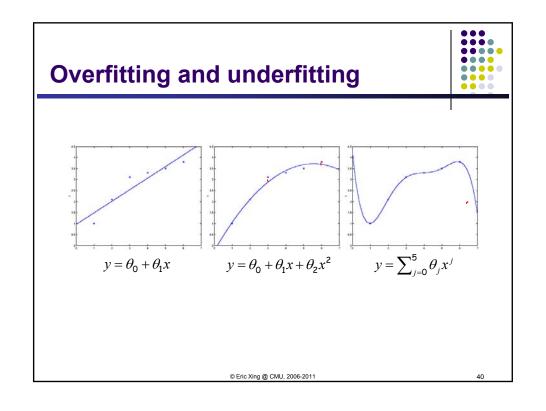
• After fit:



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

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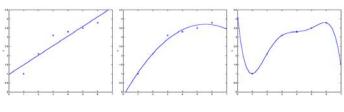




Bias and variance



- 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



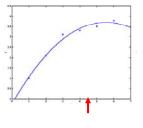
• The algorithm:

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

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

now we fit
$$\theta$$
 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 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)

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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.

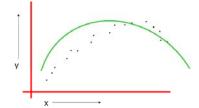
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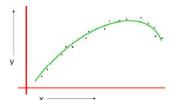
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Robust Regression



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





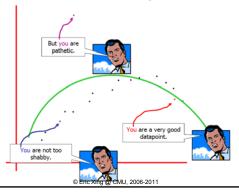
How can we do this?

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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"

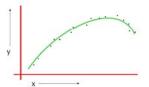


(Courtesy to Andrew Moor

Robust regression



- For k = 1 to R...
 - Let (x_k, y_k) be the kth datapoint
 - Let y^{est}_k 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:



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

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

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Robust regression—probabilistic interpretation



• What regular regression does:

Assume y_k was originally generated using the following recipe:

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

Computational task is to find the Maximum Likelihood estimation of $\boldsymbol{\theta}$

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Robust regression—probabilistic interpretation



What LOESS robust regression does:

Assume y_k was originally generated using the following recipe:

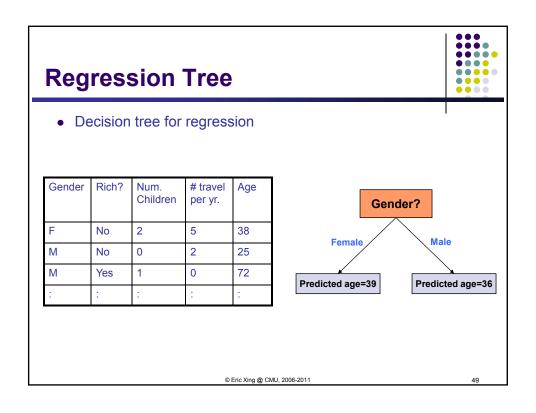
with probability
$$p$$
: $y_k = \theta^T \mathbf{x}_k + \mathcal{N}(\mathbf{0}, \sigma^2)$

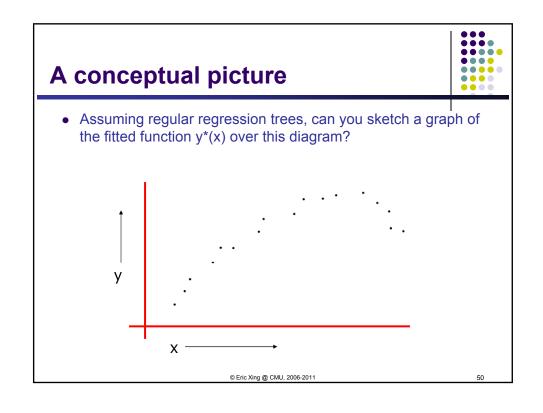
but otherwise
$$y_k \sim \mathcal{N}(\mu, \sigma_{\text{huge}}^2)$$

Computational task is to find the Maximum Likelihood estimates of θ , p, μ and $\sigma_{\rm huge}$.

 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

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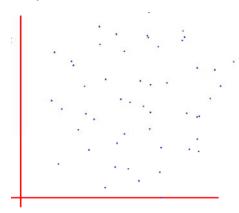




How about this one?



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
- Equivalence of LMS and MLE
- 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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