Machine Learning: Lecture I

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SLAC

CERN Academic Training Lectures

April 26-28, 2017

Lecture Structure

- Lecture I
  - What is Machine Learning
  - Linear Regression and Classification
  - Fitting a model: Cost Functions, Regularization, Gradient Descent
- Lecture II
  - Intro to Neural Networks
  - Decision Trees and ensemble methods
  - Dimensionality reduction
  - Clustering
- Lecture III – Jon Shlens (Google Brain)
  - Deep Learning, basics and current research
- Topics we won't be able to cover in such a short time
  - SVM
  - Gaussian Processes
  - Variational Inference
  - Sequence modeling, Hidden Markov Models
  - …

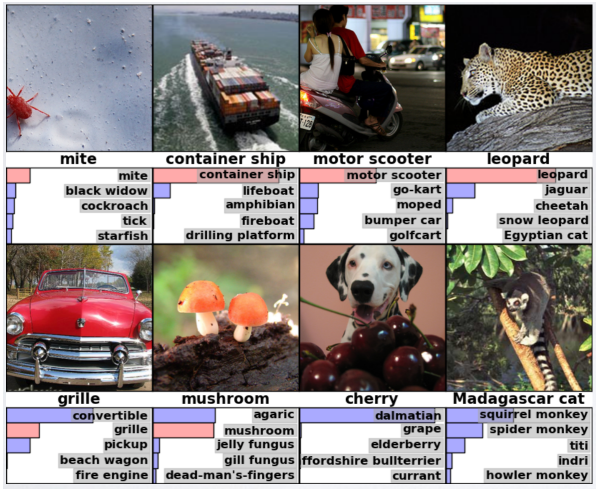
What is Machine Learning?

What is Machine Learning?

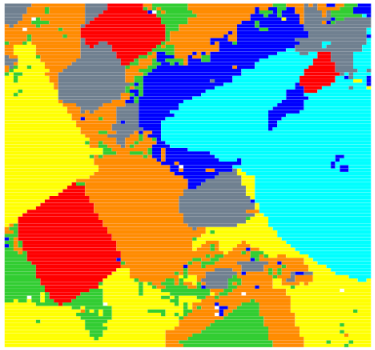
- Giving computers the ability to learn without explicitly programming them (Arthur Samuel, 1959)
- Statistics + Algorithms
- Computer Science + Probability + Optimization Techniques
- **Fitting data with complex functions**
- **Mathematical models** learnt from data that characterize the patterns, regularities, and relationships amongst variables in the system

Where is ML Used, an Incomplete List

- Natural Language Processing
- Speech and handwriting recognition
- Object recognition and computer vision
- Fraud detection
- Financial market analysis
- Search engines
- Spam and virus detection
- Medical diagnosis
- Robotics control
- Automation: energy usage, systems control, video games, self-driving cars
- Advertising
- Data Science
- …



Predicted Land Usage



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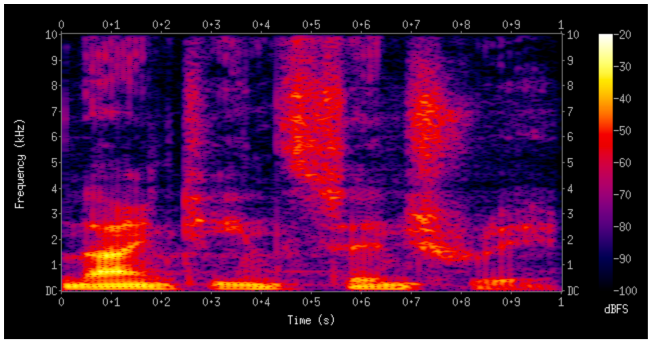

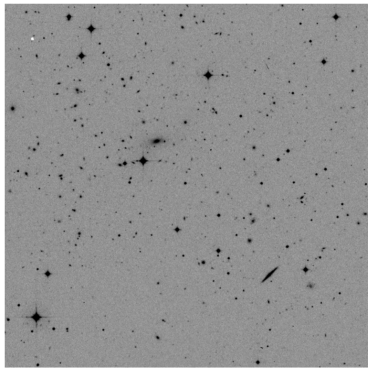

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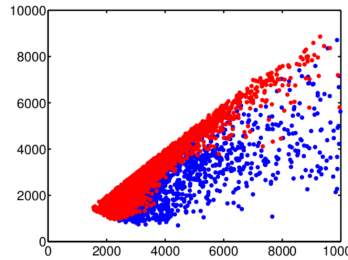
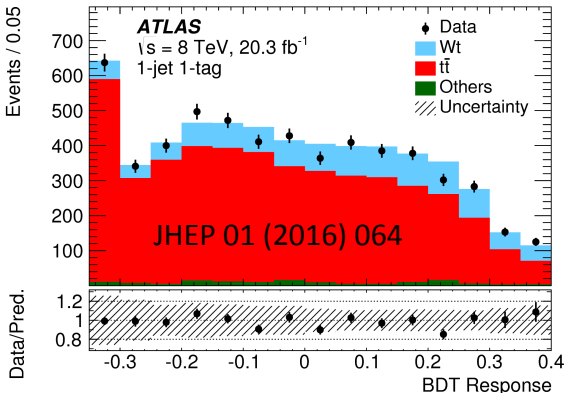
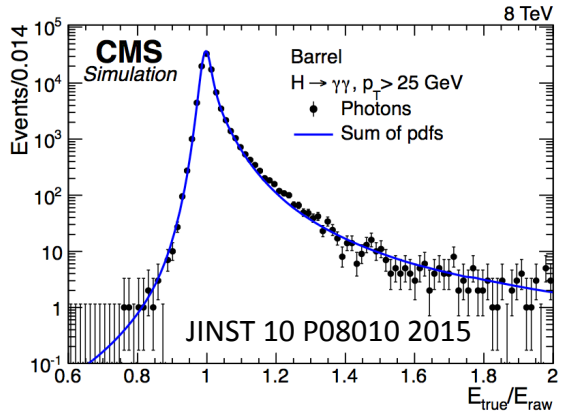


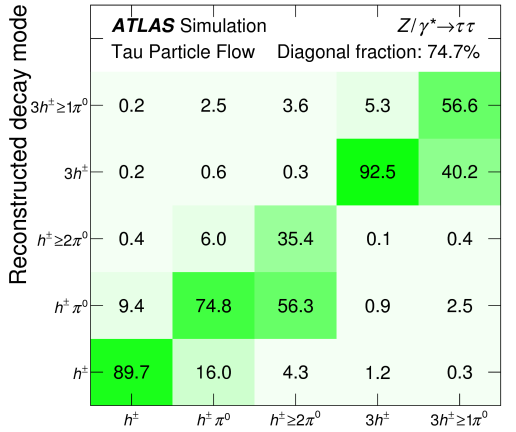
Minor elliptical axis (y) against Major elliptical axis (x) for stars (red) and galaxies (blue). (Amos Storkey)

Machine Learning Applied Widely in HEP

- **In analysis**:
  - Classifying signal from background, especially in complex final states
  - Reconstructing heavy particles and improving the energy / mass resolution
  - …
- **In reconstruction**:
  - Improving detector level inputs to reconstruction
  - Particle identification tasks
  - Energy / direction calibration
  - …
- **In the trigger**:
  - Quickly identifying complex final states
  - …
- **In computing**:
  - Estimating dataset popularity, and determining how number and location of dataset replicas
  - …







arXiv:1512.05955

Machine Learning: Models

- Key element in machine learning is a **mathematical model**
  - A mathematical characterization of system(s) of interest, typically via random variables
  - Chosen model depends on the task / available data

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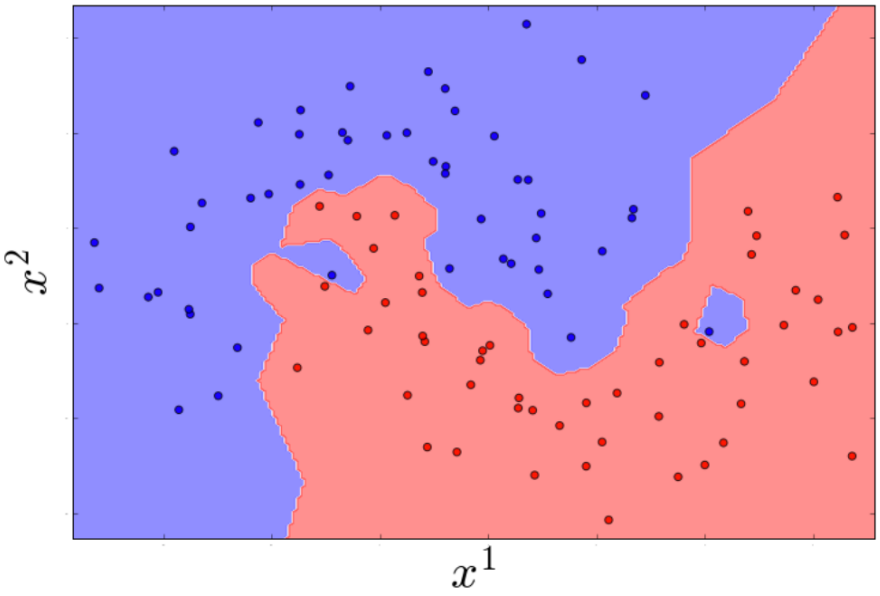

[Rogozhnikov]

Machine Learning: Models

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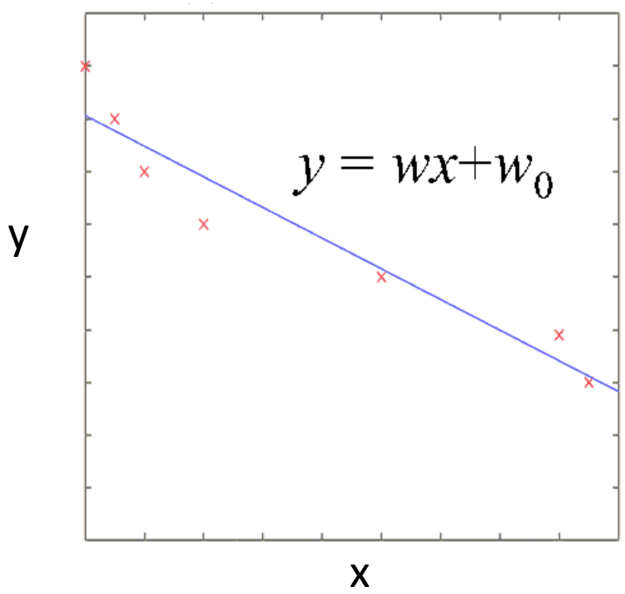

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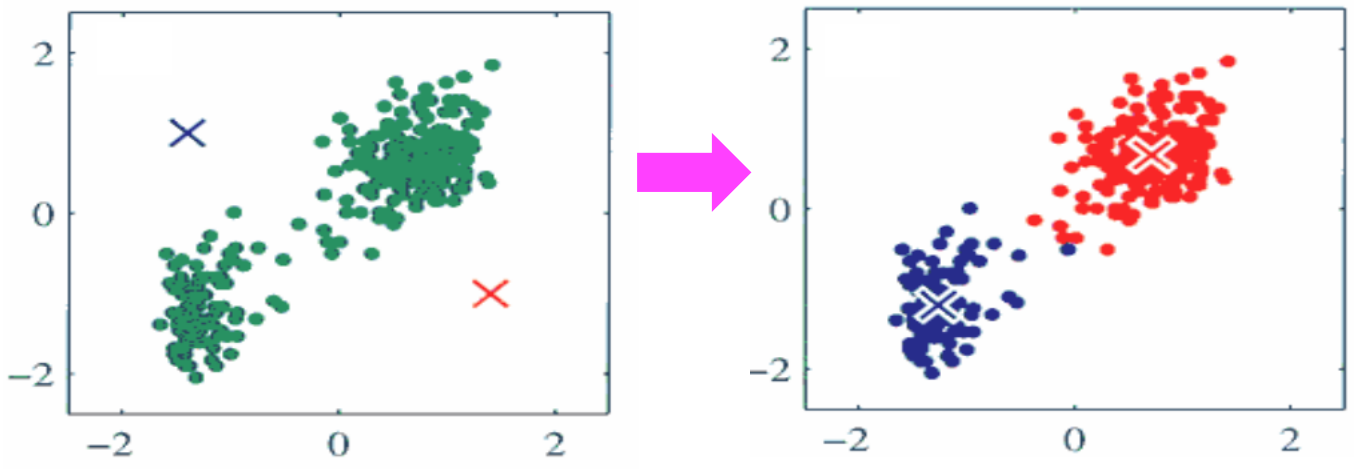

[Bishop]

Machine Learning: Models

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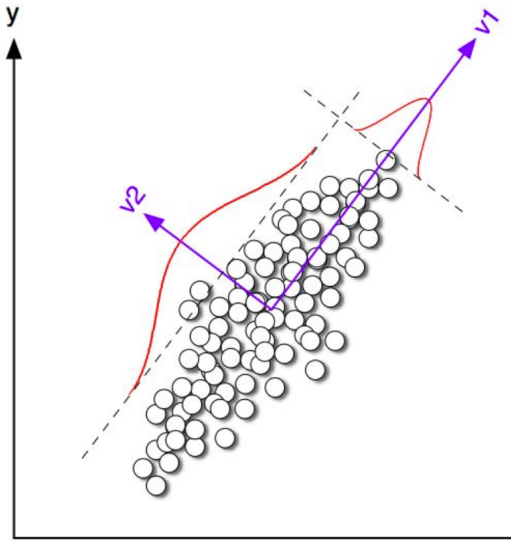
  - **Dimensionality reduction:**



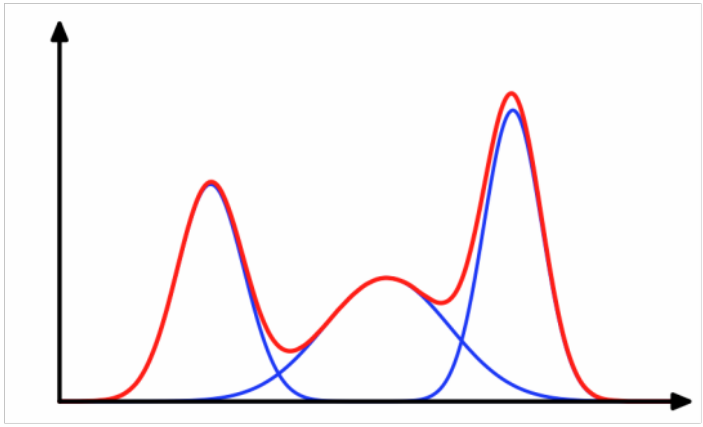
https://lazyprogrammer.me/tutorial-principal-components-analysis-pca/

Machine Learning: Models

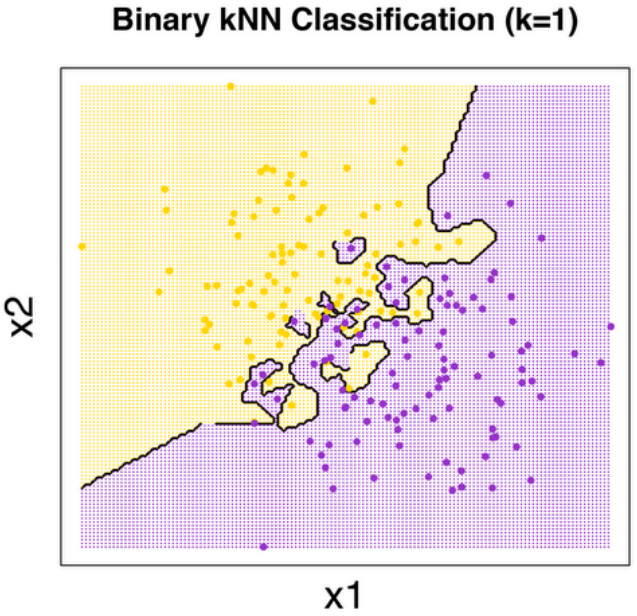
- Key element in machine learning is a **mathematical model**
  - A mathematical characterization of system(s) of interest, typically via random variables
  - Chosen model depends on the task / available data
- **Learning**: estimate statistical model from data
- **Prediction and Inference:** using statistical model to make predictions on new data points and infer properties of system(s)

Parametric vs. Non-parametric Models

- **Parametric Models**: models that do not grow in complexity with dataset size. Fixed set of parameters to learn
  - Example: sum of Gaussians, each with mean, variance, and normalization

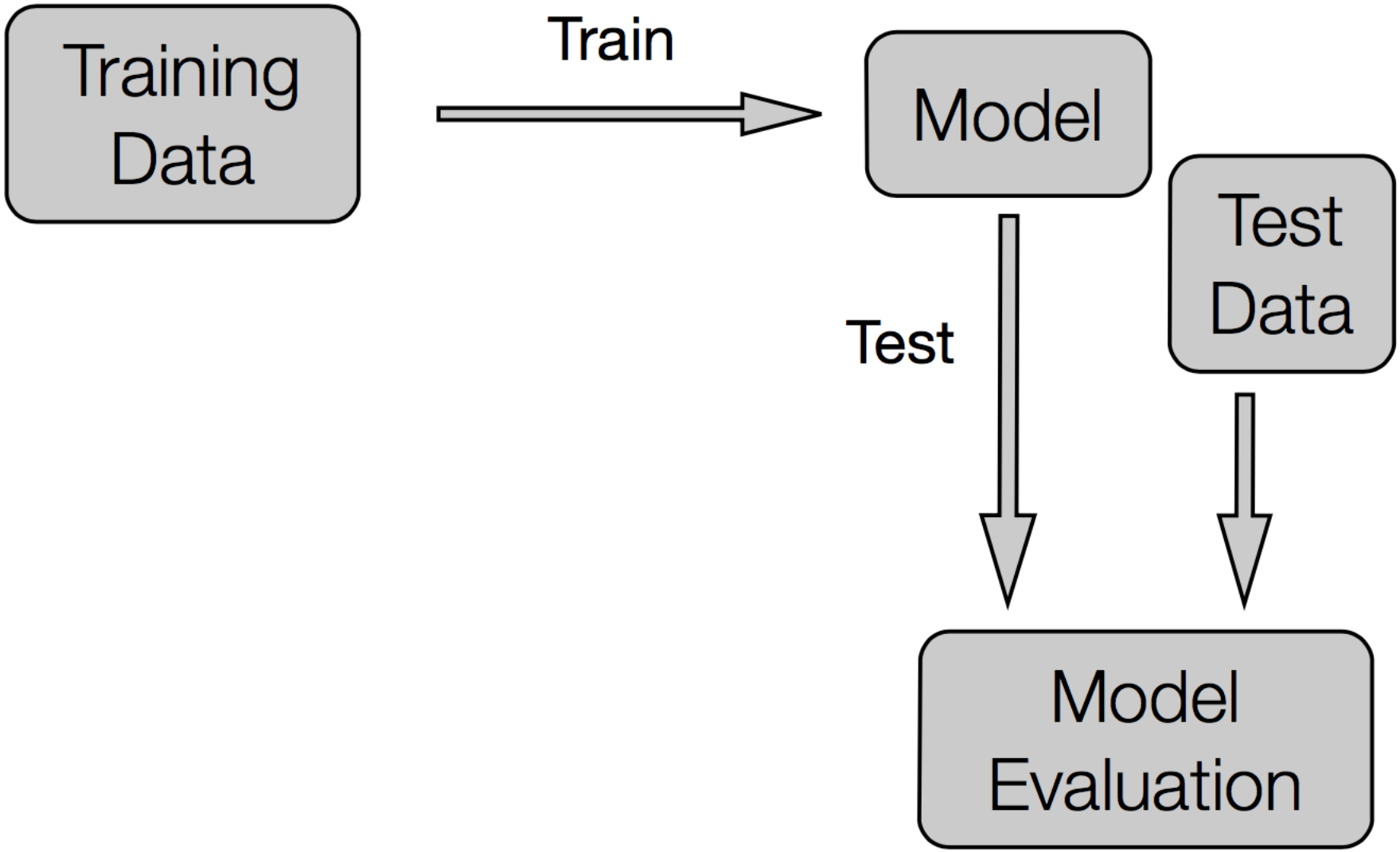


- **Non-Parametric Models**: models that do not have a fixed set of parameters, often grow in complexity with more data
  - Example: model predictions of a new data point using nearest known datapoint. The more known datapoints, the more complex is the model



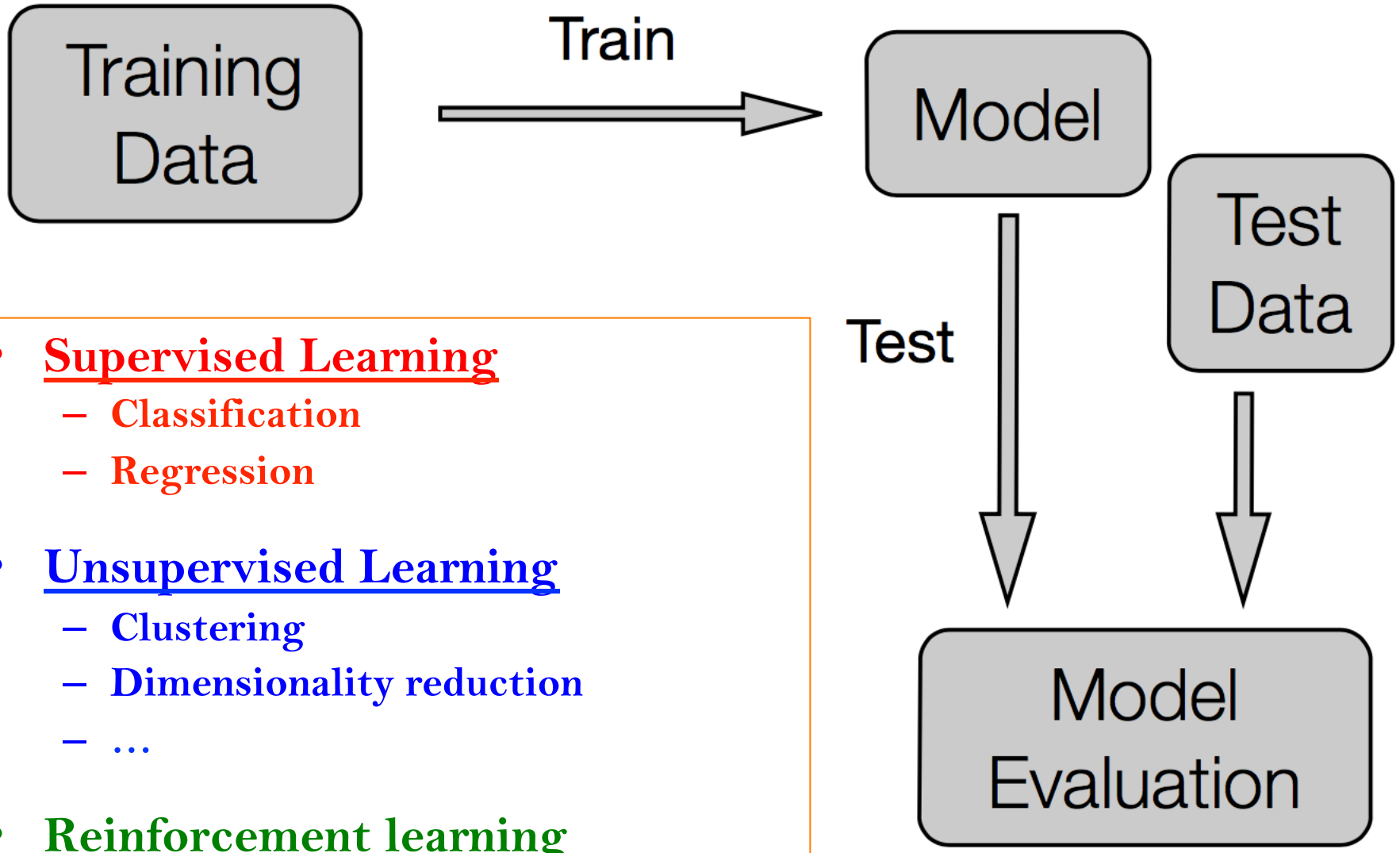
http://bdewilde.github.io/blog/blogger/2012/10/26/classification-of-hand-written-digits-3/

Learning



[Ravikumar]

Learning



- **Supervised Learning**
  - Classification
  - Regression
- **Unsupervised Learning**
  - Clustering
  - Dimensionality reduction
  - …
- **Reinforcement learning**

[Ravikumar]

Notation

- $\mathbf{X} \in \mathbb{R}^{mxn}$ Matrices in bold upper case:
- $\mathbf{x} \in \mathbb{R}^{n(x1)}$ Vectors in bold lower case
- $x \in \mathbb{R}$ Scalars in lower case, non-bold
- $\mathcal{X}$ Sets are script
- $\{\mathbf{x}_i\}_1^m$ Sequence of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$
- $y \in \mathbb{I}^{(k)}$ / $\mathbb{R}^{(k)}$ Labels represented as
  - Integer for classes, often {0,1}. E.g. {Higgs, Z}
  - Real number. E.g electron energy

- Variables = features = inputs
- Data point $\mathbf{x} = \{x_1, \ldots, x_n\}$ has n-features

- Typically use affine coordinates:

$$y = \mathbf{w}^T\mathbf{x} + w_0 \rightarrow \mathbf{w}^T\mathbf{x}$$
$$\rightarrow \mathbf{w} = \{w_0, w_1, \ldots, w_n\}$$
$$\rightarrow \mathbf{x} = \{1, x_1, \ldots, x_n\}$$

Probability Review

- Joint distribution of two variables: p(x,y)
- Conditional distribution: $p(y|x) = \frac{p(x,y)}{p(x)}$
- Bayes theorem: $p(y|x) = \frac{p(x|y)p(y)}{p(x)}$
- Expected value: $\mathbf{E}[f(x)] = \int f(x)p(x)\mathrm{d}x$
- Normal distribution:
  - $x \sim N(\mu, \sigma) \rightarrow p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$

Supervised Learning

- Given N examples with features $\{x_i \in \mathcal{X}\}$ and **targets** $\{y_i \in \mathcal{Y}\}$, learn function mapping **h(x)=y**
  - **Classification**: $\mathcal{Y}$ is a finite set of **labels** (i.e. classes)

$\mathcal{Y} = \{0, 1\}$ for **binary classification**,
encoding classes, e.g. Higgs vs Background

$\mathcal{Y} = \{c_1, c_2, \ldots c_n\}$ for **multi-class classification**

represent with "**one-hot-vector**"

$\rightarrow$ $y_i = (0, 0, \ldots, 1, \ldots 0)$

were k^{th} element is 1 and all others zero for class c_k

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  - **Regression**: $\mathcal{Y}$ = Real Numbers
- Often these are **discriminative models**, in which case we model:

$$h(x) = p(y \mid x)$$

- Sometimes use **generative models**, estimate joint distribution p(y, x)
  - Often estimate class conditional density p(x | y) and prior p(y)
  - Use Bayes theorem to then compute:

$$h(\mathbf{x}) = p(y|\mathbf{x}) \propto p(\mathbf{x}|y)p(y)$$

Unsupervised Learning

- Given some data $D=\{x_i\}$, but no labels, find structure in the data

  - **Clustering**: partition the data into groups $D=\{D_1 \cup D_2 \cup D_3 \ldots \cup D_k\}$

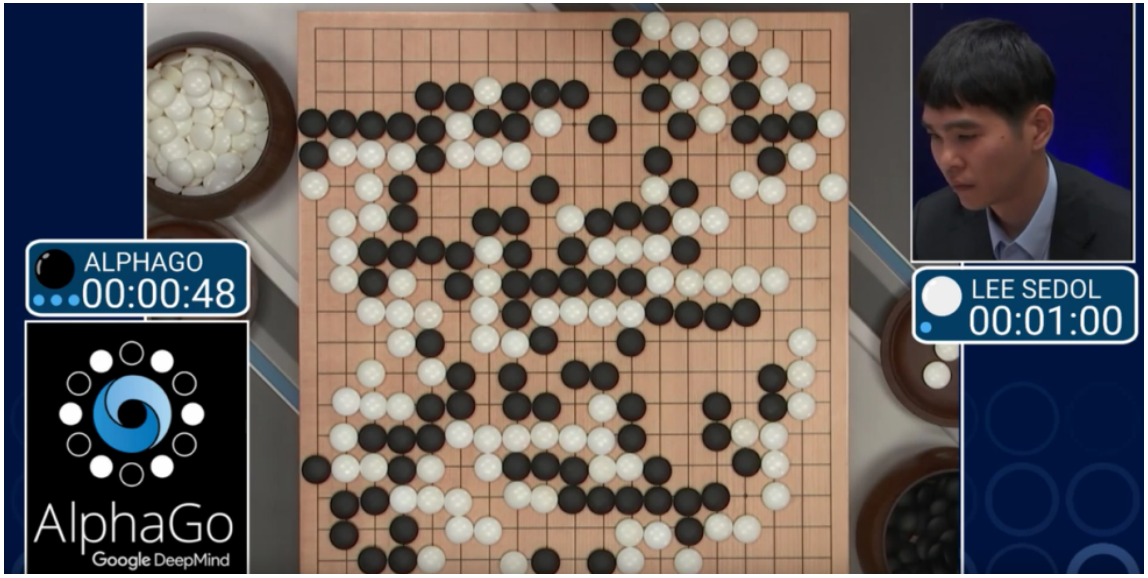
  - **Dimensionality reduction**: find a low dimensional (less complex) representation of the data with a mapping $Z=h(X)$

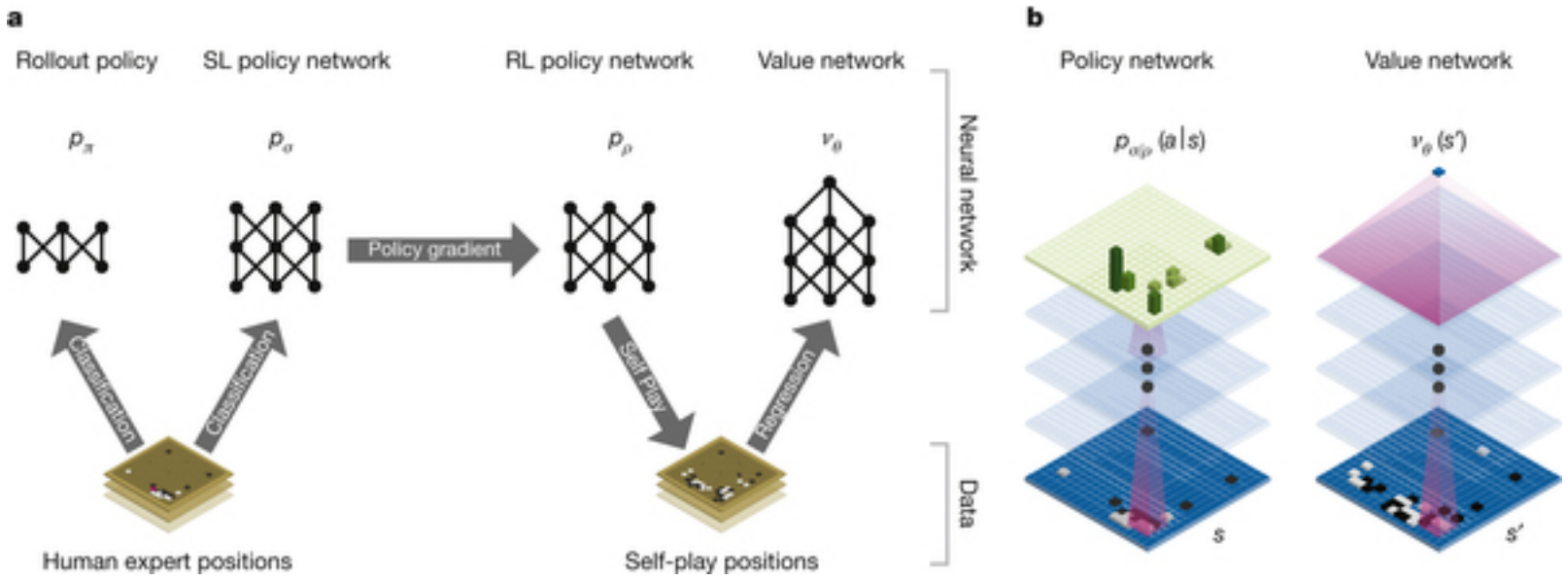
Reinforcement Learning

[Ravikumar]

- Models for agents that take actions depending on current state
  - Actions incur rewards, and affect future states ("feedback")
- Learn to make the best sequence of decisions to achieve a given goal when feedback is often delayed until you reach the goal

Deep Reinforcement Learning with AlphaGo





Nature 529, 484–489 (28 January 2016)

Supervised Learning: How does it work?

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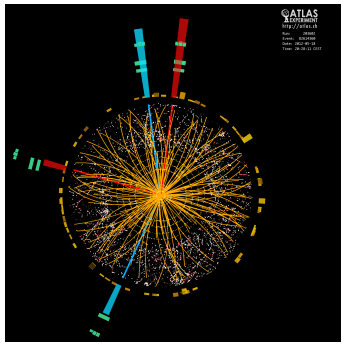


h(**x**; **w**)
Function with adjustable parameters

Loss Function

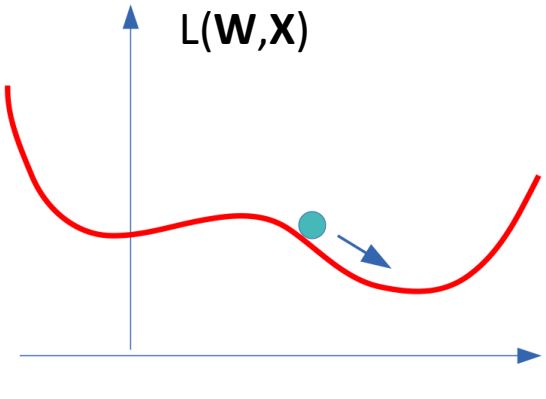
Compare prediction with true label

Loss

True labels:
Higgs = 1
Bkg = 0

- Design function with adjustable parameters
- Design a Loss function
- Find best parameters which minimize loss

Y. Le Cun



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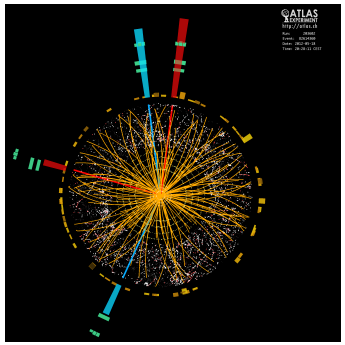

h(**x**; **w**)
Function with adjustable parameters

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Compare prediction with true label

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True labels:
Higgs = 1
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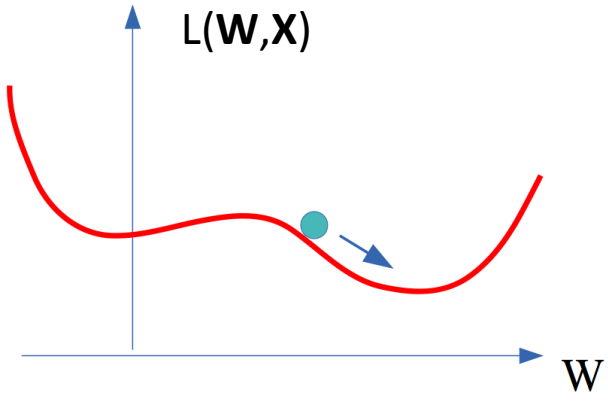
- Design function with adjustable parameters
- Design a Loss function
- Find best parameters which minimize loss
  - Use a labeled *training-set* to compute loss
  - Adjust parameters to reduce loss function
  - Repeat until parameters stabilize
- Estimate final performance on *test-set*

Y. Le Cun



Empirical Risk Minimization

$$\arg\min_{\mathbf{w}} \underbrace{\frac{1}{N}\sum_{i=1}^{N} L(h(\mathbf{x}_i;\mathbf{w}), y_i)}_{\text{Average expected loss}} + \underbrace{\lambda\Omega(\mathbf{w})}_{\text{Model regularization}}$$

- Framework to design learning algorithms
  - L(…) is a loss function comparing prediction h(…) with target y
  - $\Omega(\mathbf{w})$ is a regularizer, penalizing certain values of $\mathbf{w}$
    - λ controls how much we penalize, and is a hyperparameter that we have to tune
    - We will come back to this later
- Learning is cast as an optimization problem

Example Loss Functions

- Square Error Loss:
  - Often used in regression

$$L(h(\mathbf{x};\mathbf{w}),y) = \big(h(\mathbf{x};\mathbf{w}) - y\big)^2$$

- Cross entropy:
  - With y ∈ {0,1}
  - Often used in classification

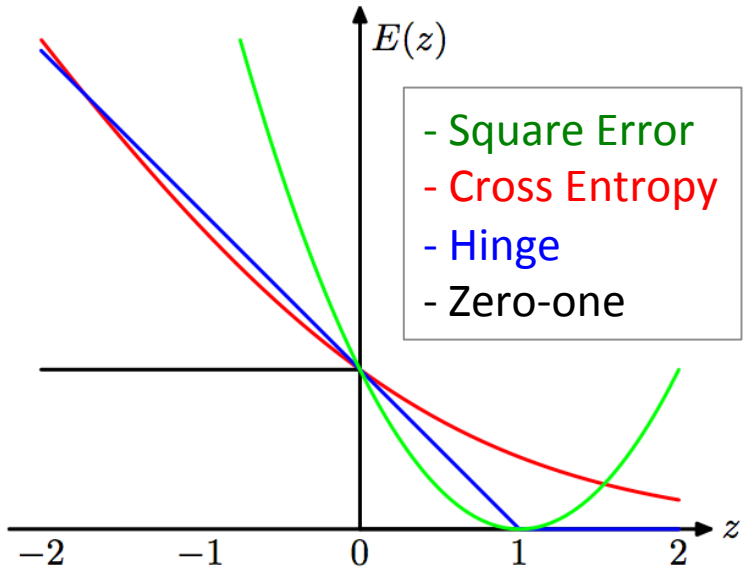
$$L(h(\mathbf{x};\mathbf{w}),y) = -\,y \log h(\mathbf{x};\mathbf{w}) - (1-y)\log(1-h(\mathbf{x};\mathbf{w}))$$

- Hinge Loss:
  - With y ∈ {-1,1}

$$L(h(\mathbf{x};\mathbf{w}),y) = \max(0, 1 - yh(\mathbf{x};\mathbf{w}))$$

- Zero-One loss
  - With h(**x**; **w**) predicting label

$$L(h(\mathbf{x};\mathbf{w}),y) = 1_{y \neq h(\mathbf{x};\mathbf{w})}$$



[Bishop]

Maximum Likelihood

- Describe a process behind the data
- Write down the likelihood of the observed data

$$\mathcal{L}(\mathbf{w}) = p(\mathbf{y}|\mathbf{X};\mathbf{w}) = \prod_i p(y_i|\mathbf{x}_i;\mathbf{w})$$

  - Where second equality holds if data is independent and identically distributed
  - Often minimize negative-log-likelihood for numerical stability
    - Same as maximizing likelihood since log is monotonic and differentiable away from zero

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$$\mathcal{L}(\mathbf{w}) = p(\mathbf{y}|\mathbf{X};\mathbf{w}) = \prod_i p(y_i|\mathbf{x}_i;\mathbf{w})$$

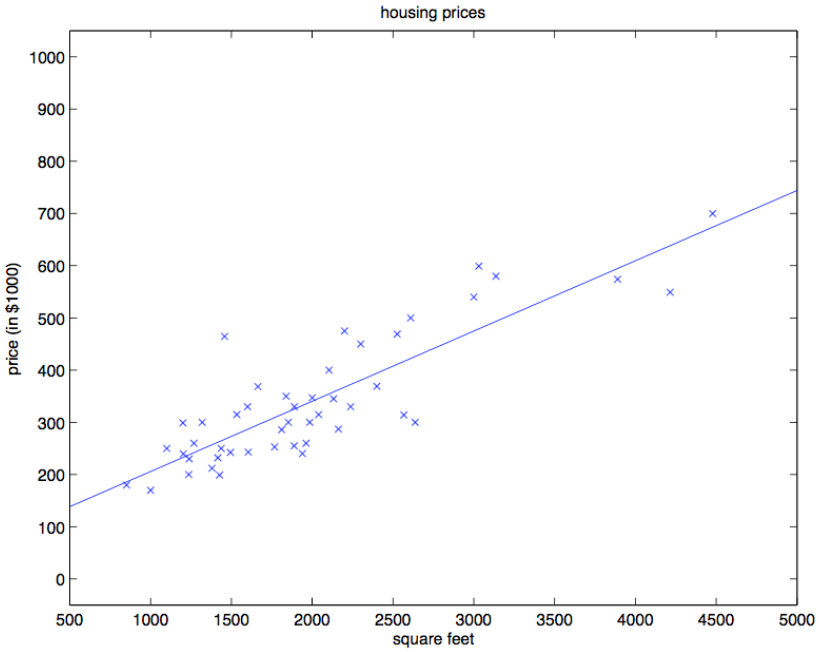
- Select parameters that make data most likely
  - General strategy for parameter estimation

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \mathcal{L}(\mathbf{w}) = \arg\min_{\mathbf{w}} -\ln \mathcal{L}(\mathbf{w}) = \arg\min_{\mathbf{w}} -\sum_i \ln p(y_i|\mathbf{x}_i;\mathbf{w})$$

Linear Methods

Least Squares Linear Regression

- Set of input / output pairs $D = \{\mathbf{x}_i , y_i\}_{i=1\ldots n}$
  - $\mathbf{x}_i \in \mathbb{R}^m$
  - $y_i \in \mathbb{R}$



- Assume a linear model

$$h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T\mathbf{x}$$

- Squared Loss function:

$$L(\mathbf{w}) = \frac{1}{2}\sum_i \left(y_i - h(\mathbf{x}_i; \mathbf{w})\right)^2$$

- Find $\mathbf{w}^* = \arg\min_{\mathbf{w}} L(\mathbf{w})$

Least Squares Linear Regression: Matrix Form

- Set of input / output pairs $D = \{\mathbf{x}_i , y_i\}_{i=1\ldots n}$
  - Design matrix $\mathbf{X} \in \mathbb{R}^{nxm}$
  - Target vector $\mathbf{y} \in \mathbb{R}^{n}$

$$\mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,m} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,m} \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

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- Rewrite loss: $$L(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{X}\mathbf{w})^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$

- Minimize w.r.t. $\mathbf{w}$: $$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \arg\min_{\mathbf{w}} L(\mathbf{w})$$

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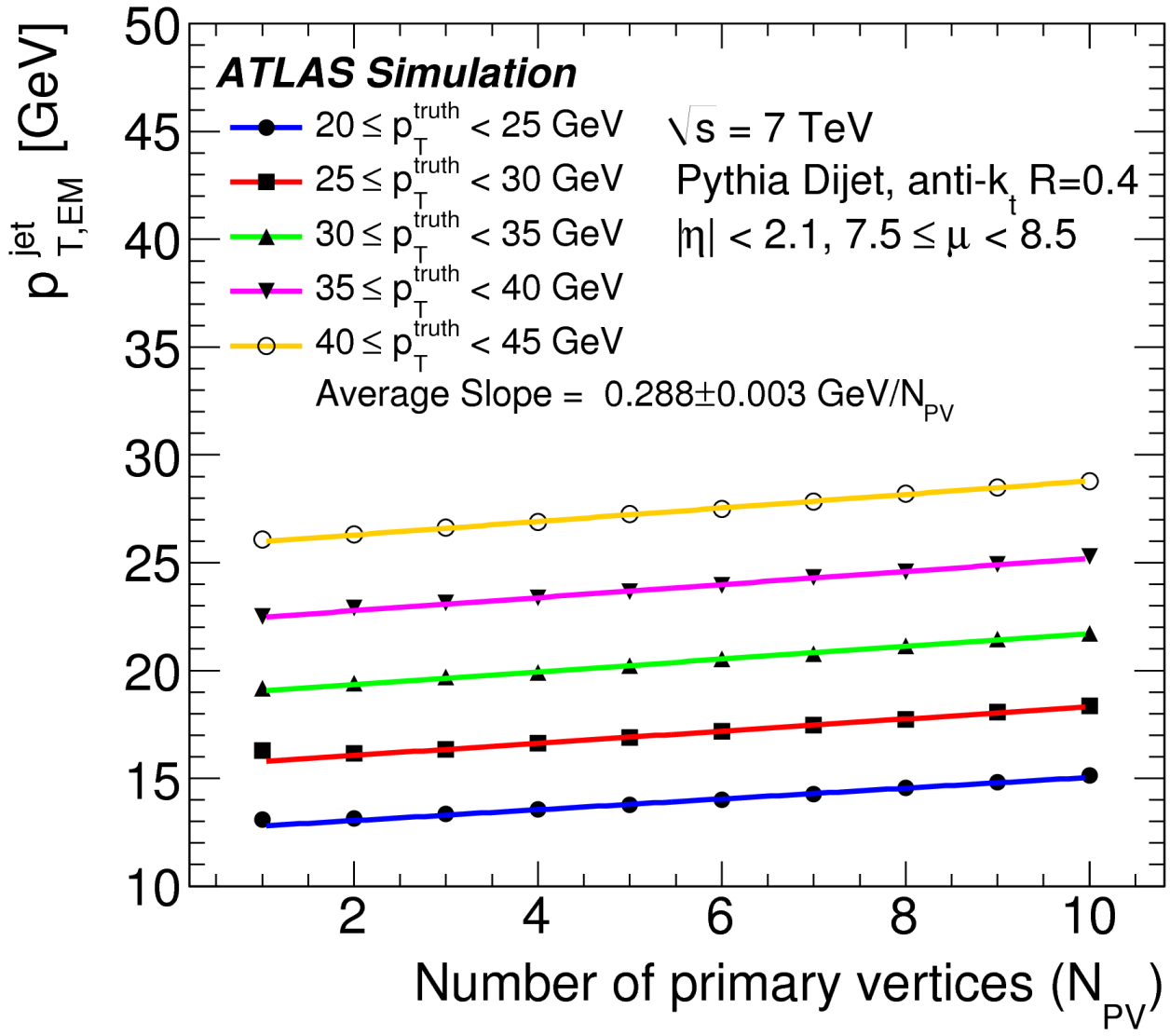
- What if we have correlated variables? *Multi-collinearity*
  - $\mathbf{X}$ is close to singular
  - Inverse is highly sensitive to random errors

- Hint: Regularization can help!

Linear Regression Example

Eur. Phys. J. C (2015) 75:17



- Reconstructed Jet energy vs. Number of primary vertices

Linear Regression – Probabilistic Interpretation

- Assume $y_i = mx_i + e_i$
- Random error: $e_i \sim \mathcal{N}(0, \sigma) \rightarrow p(e_i) \propto \exp\left(\frac{1}{2}\frac{e_i^2}{\sigma^2}\right)$
  - Noisy measurements, unmeasured variables, …

Linear Regression – Probabilistic Interpretation

- Assume $y_i = mx_i + e_i$
- Random error: $e_i \sim \mathcal{N}(0, \sigma) \rightarrow p(e_i) \propto \exp\left(\frac{1}{2}\frac{e_i^2}{\sigma^2}\right)$
  - Noisy measurements, unmeasured variables, …
- Then $y_i \sim \mathcal{N}(mx_i, \sigma) \rightarrow p(y_i|x_i; m) \propto \exp\left(\frac{1}{2}\frac{(y_i - mx_i)^2}{\sigma^2}\right)$

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$$L(m) = p(\mathbf{y}|\mathbf{X}; m) = \prod_i p(y_i|x_i; m)$$

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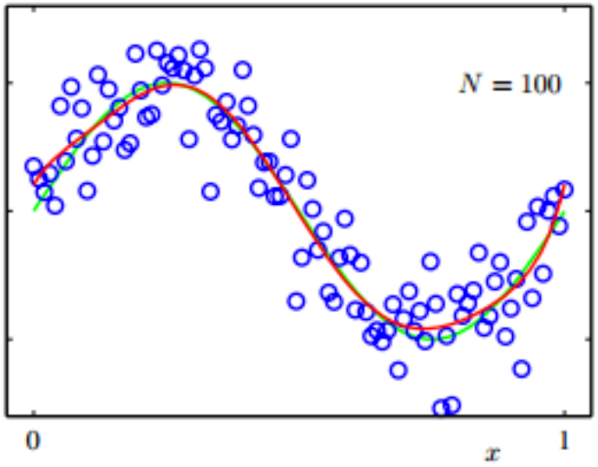
Squared loss function!

Why Take a Probabilistic Approach?

- Allows us to get calibrated estimates of $p(y|\mathbf{x})$
- Separates predictions from modeling
- A general framework for parameter estimation.
  - Can use to fit other parameters of the model.

Basis Functions



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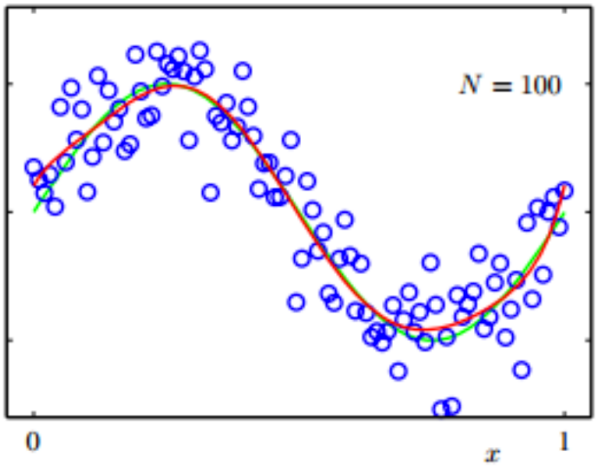
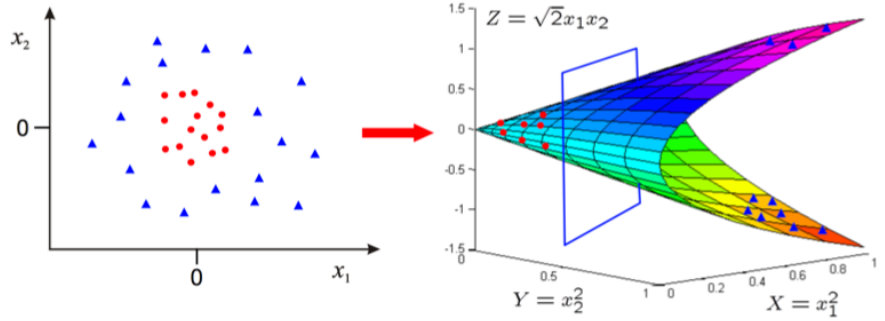
Basis Functions



$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \quad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

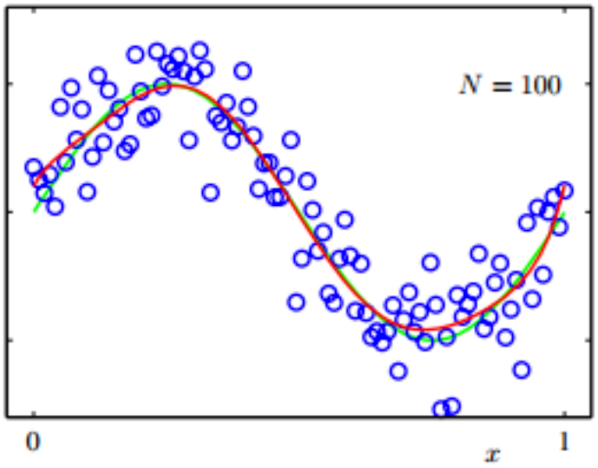


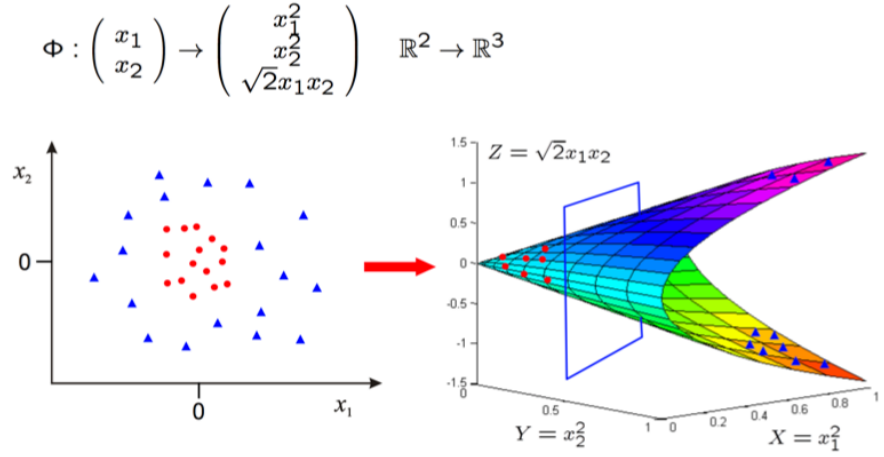
- What if non-linear relationship between **y** and **x**?
- Can choose basis functions $\phi(x)$ to form new features

$$\mathbf{y}_i = \mathbf{w}^T \phi(x_i)$$

  - Polynomial basis $\phi(x) \sim \{1, x, x^2, x^3, \ldots\}$, Gaussian basis, …
  - **Linear regression on new features $\phi(x)$**

Basis Functions





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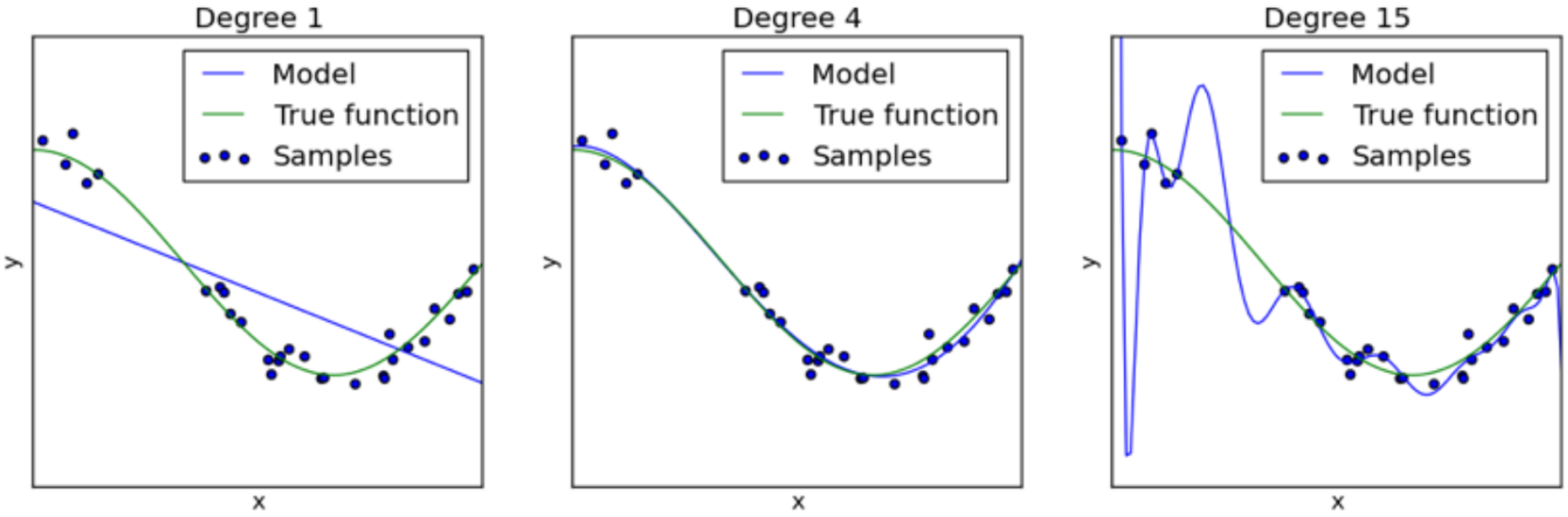
- What basis functions to choose? *Overfit* with too much flexibility?

What is Overfitting



Underfitting

Overfitting

http://scikit-learn.org/

- What models allow us to do is **generalize** from data
- Different models generalize in different ways

Bias Variance Tradeoff

- generalization error = systematic error + sensitivity of prediction
  (bias) (variance)

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- Complex models over-fit: will not deviate systematically from data (low bias) but will be very sensitive to data (high variance).

Bias Variance Tradeoff

- Model h(x), defined over dataset, modeling random variable output y

$$E[y] = \bar{y}$$
$$E[h(x)] = \bar{h}(x)$$

- Examining generalization error at x, w.r.t. possible training datasets

$$\begin{aligned} E[(y - h(x))^2] = E[(y - \bar{y})^2] &+ (\bar{y} - \bar{h}(x))^2 &+ E[(h(x) - \bar{h}(x))^2] \\ = \text{noise} &+ (\text{bias})^2 &+ \text{variance} \end{aligned}$$

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Intrinsic noise in system or measurements
Can not be avoided or improved with modeling
Lower bound on possible noise

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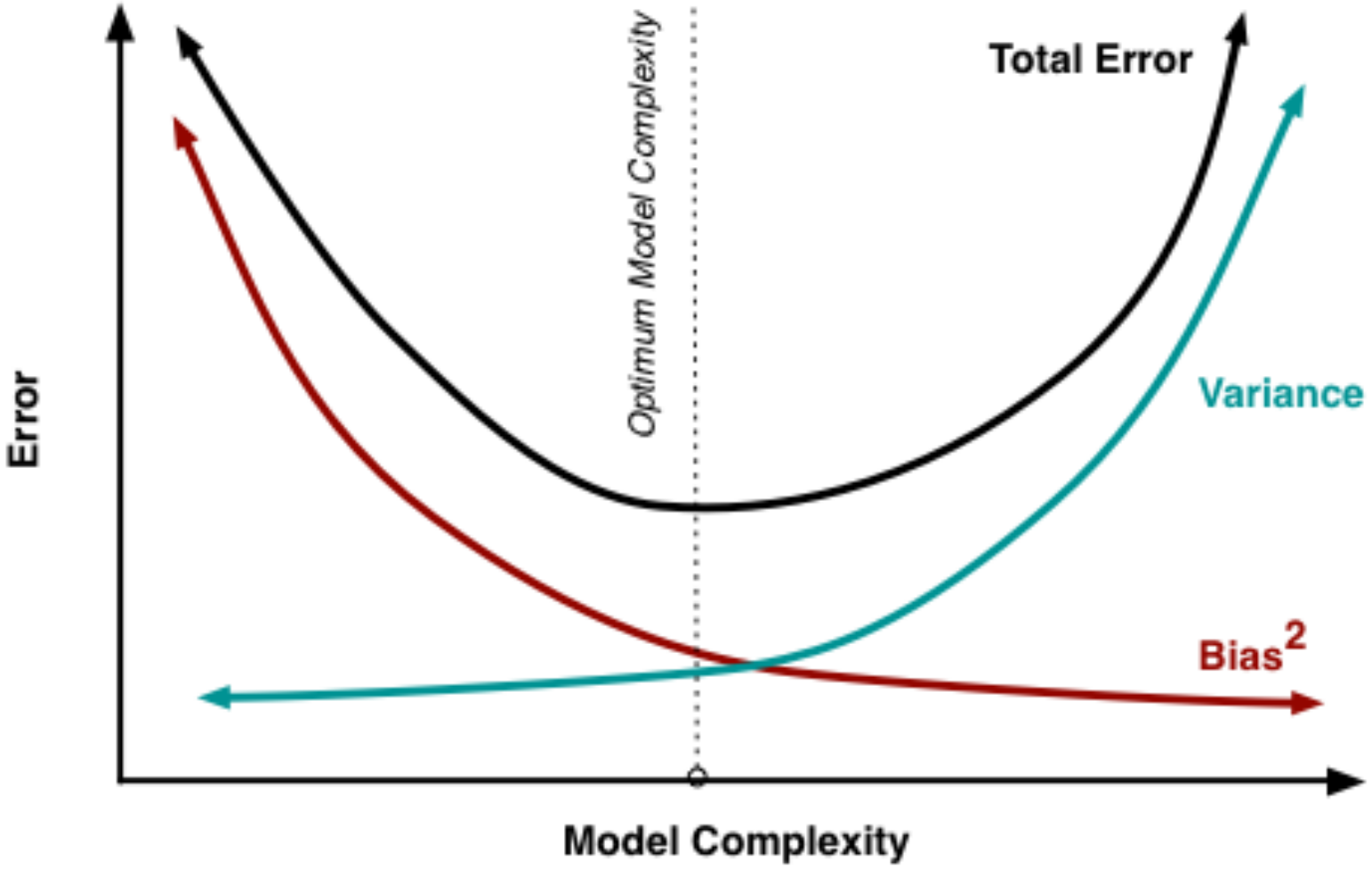
- **More Complexity** will make the model "move" more to capture the data points, and hence its **variance will be larger**.
  - **As dataset size grows, can reduce variance! Can use more complex model**

Bias Variance Tradeoff



Regularization

- Can control the complexity of a model by placing **constraints on the model parameters**
  - Trading some bias to reduce model variance

- **L2 norm**: $\Omega(\mathbf{w}) = ||\mathbf{w}||^2 = \sum_i w_i^2$
  - "Ridge regression", enforcing weights not too large
  - Equivalent to Gaussian prior over weights

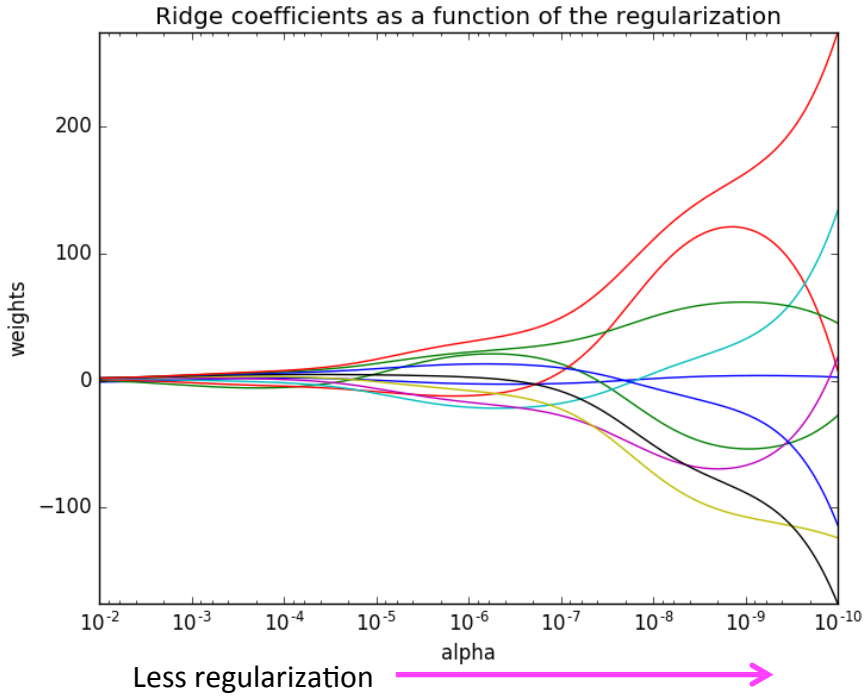
- **L1 norm**: $\Omega(\mathbf{w}) = ||\mathbf{w}|| = \sum_i |w_i|$
  - "Lasso regression", enforcing sparse weights

- Elastic net → L1 + L2 constraints

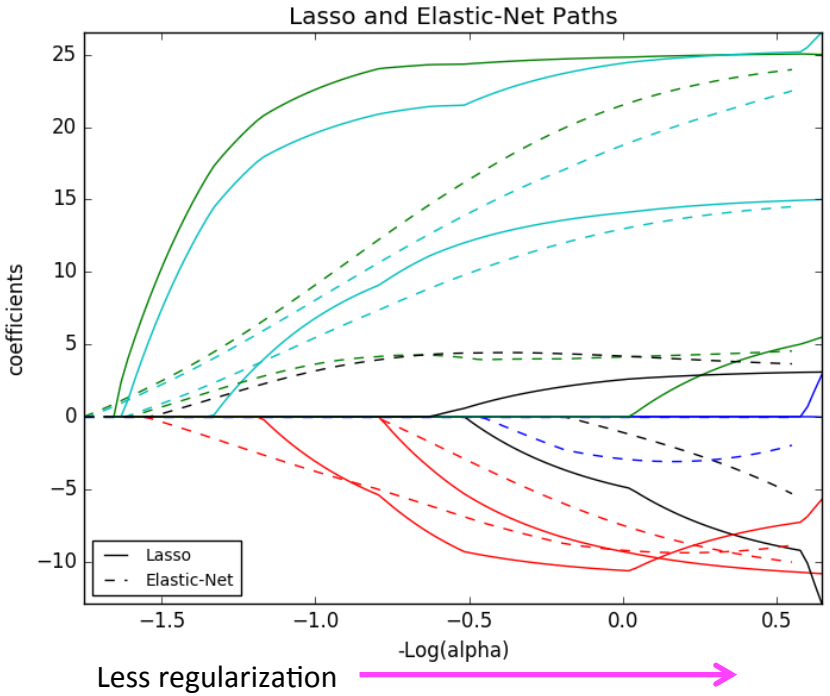
Regularized Linear Regression

$$L(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{X}\mathbf{w})^2 + \alpha\Omega(\mathbf{w})$$

$$L2: \quad \Omega(\mathbf{w}) = ||\mathbf{w}||^2$$



$$L1: \quad \Omega(\mathbf{w}) = ||\mathbf{w}||$$



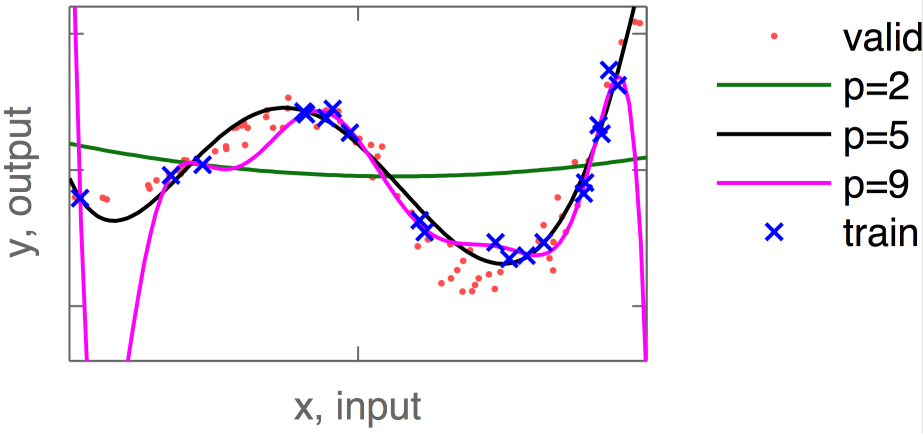
- L2 keeps weights small, L1 keeps weights sparse!
- But how to choose hyperparameter α?

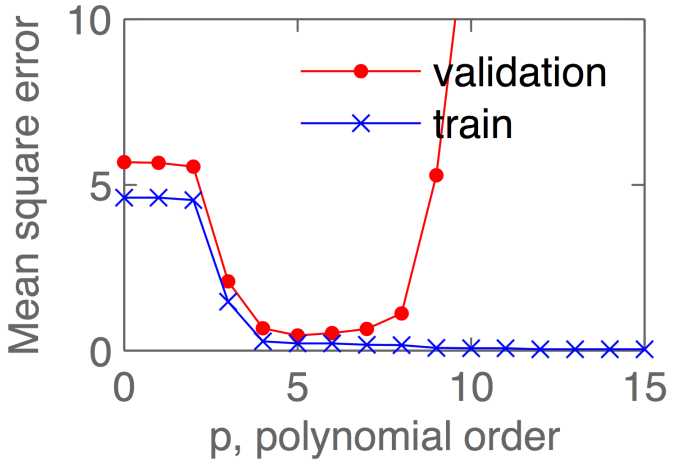
http://scikit-learn.org/

How to Measure Generalization Error?

Training set	Validation set	Test set

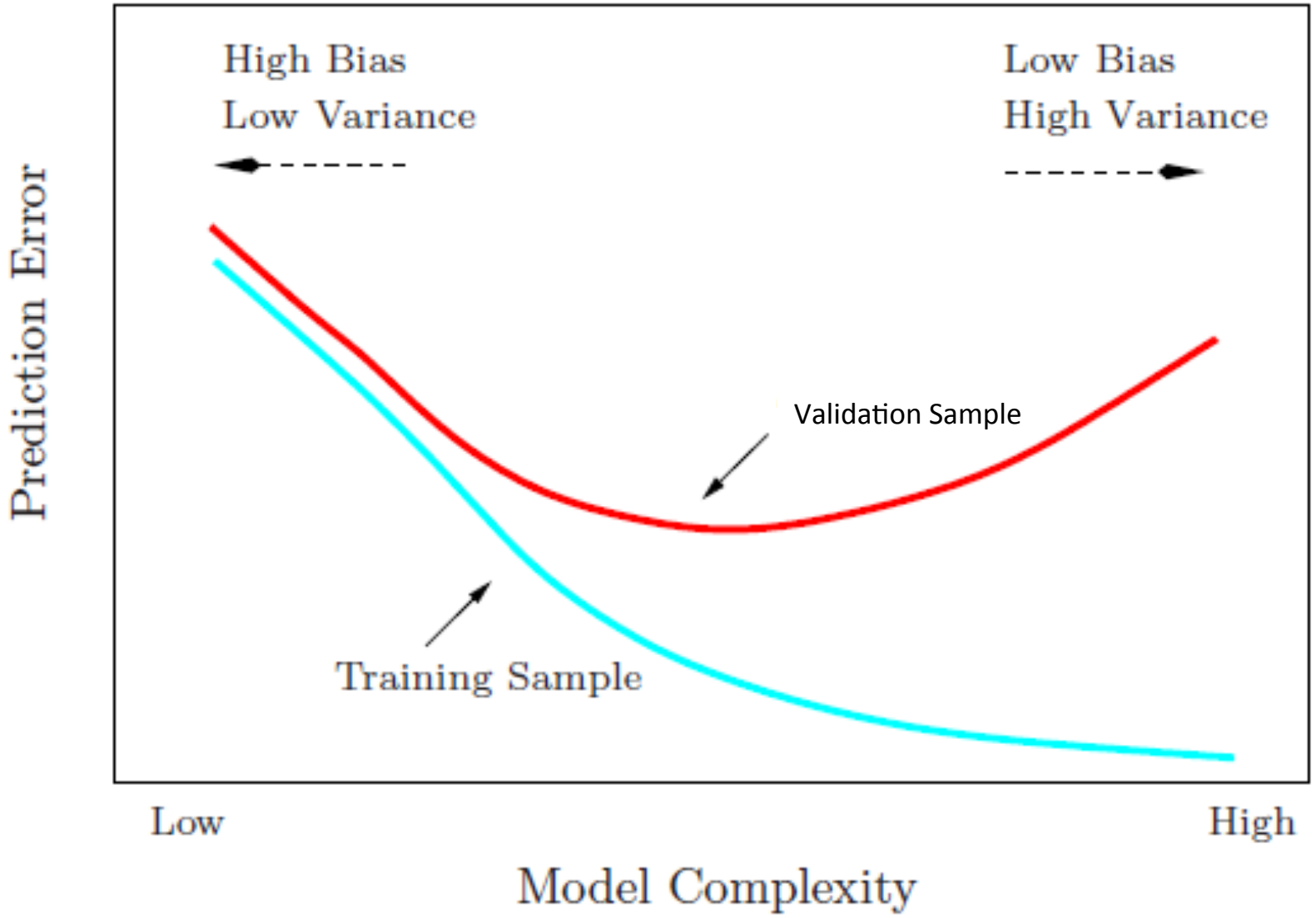
- Split dataset into multiple parts
- **Training set**
  - Used to fit model parameters
- **Validation set**
  - Used to check performance on independent data and tune hyper parameters
- **Test set**
  - final evaluation of performance after all hyper-parameters fixed
  - Needed since we tune, or "peek", performance with validation set



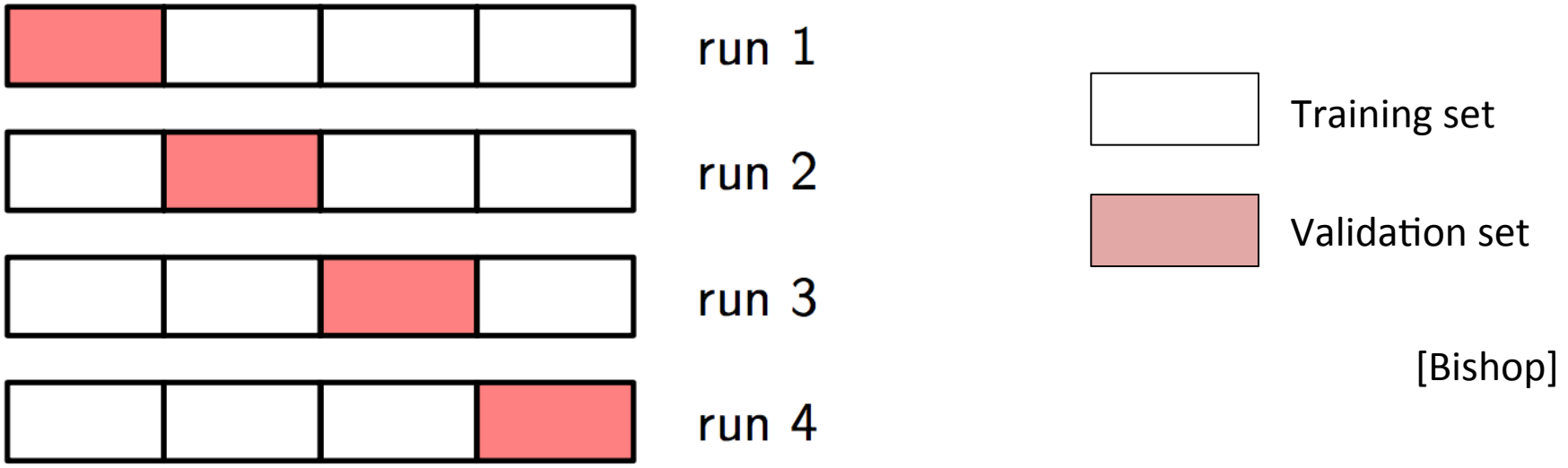


[Murray]

How to Measure Generalization Error?



Cross Validation

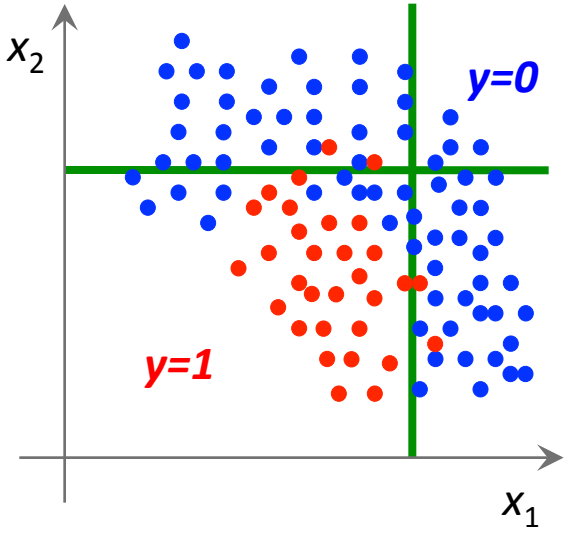


[Bishop]

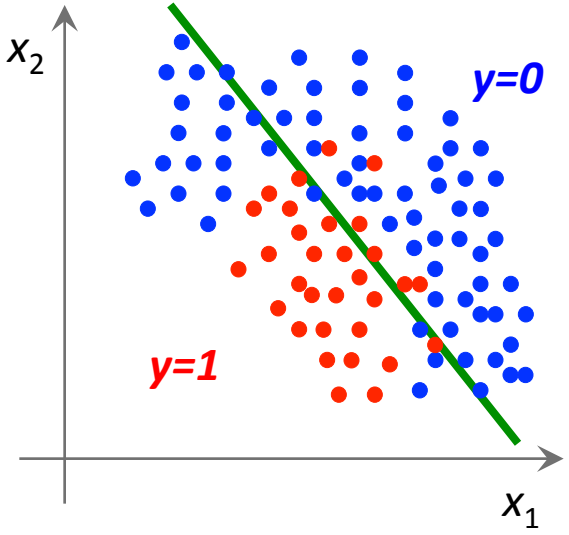
- Especially when dataset is small, split training set into K-folds
  - Train on (K-1) folds, validate on 1 fold, then iterate
  - Use average estimated performance on K-folds
  - Allows for estimate of performance RMS
- Even when dataset not small, useful technique to estimate variance of expected performance, and for comparing different models / hyperparameters

Classification

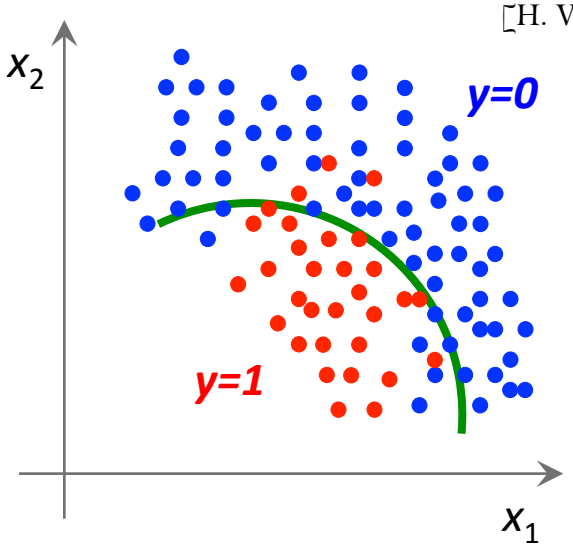
[H. Voss]



Rectangular cuts

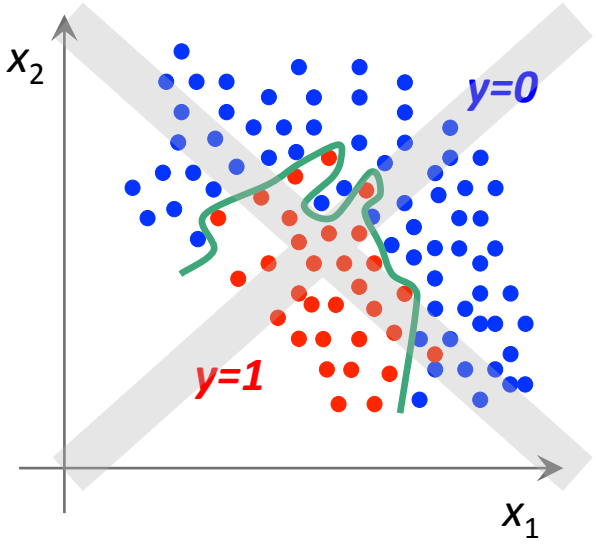


Linear discriminant



Nonlinear discriminant

- Learn a function to separate different classes of data
- Avoid over-fitting:
  - Learning too fined details about your training sample that will not generalize to unseen data

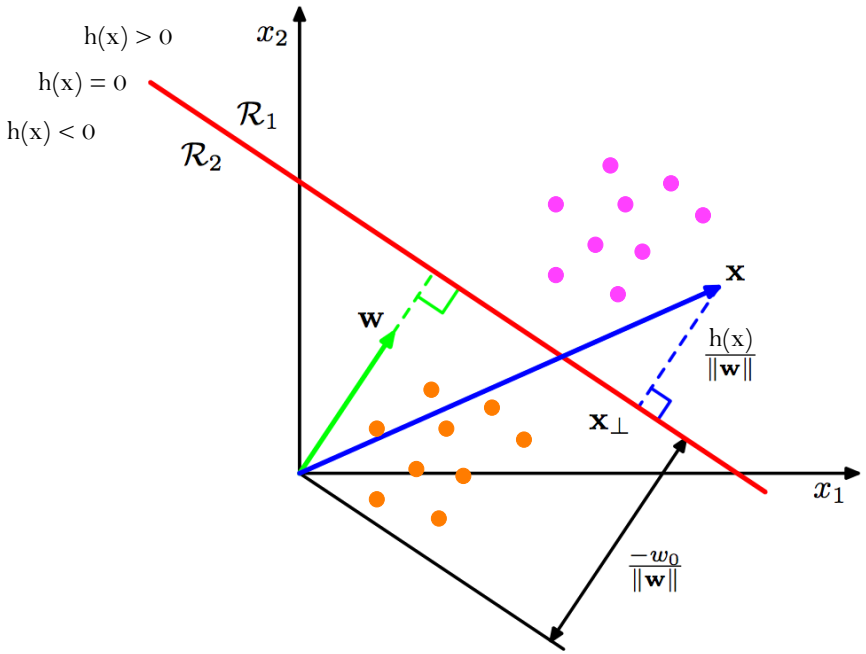


Linear Decision Boundaries

- Separate two classes:
  - $\mathbf{x}_i \in \mathbb{R}^m$
  - $y_i \in \{-1,1\}$

- Linear discriminant model

$$h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T\mathbf{x}$$



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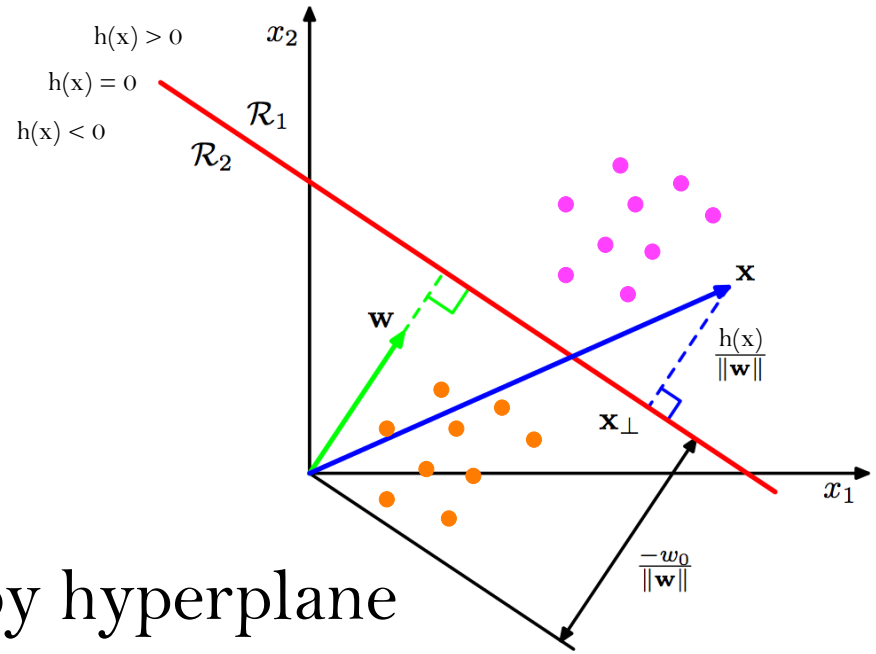


- Linear discriminant model

$$h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T\mathbf{x}$$

- **Decision boundary** defined by hyperplane

$$h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T\mathbf{x} = 0$$

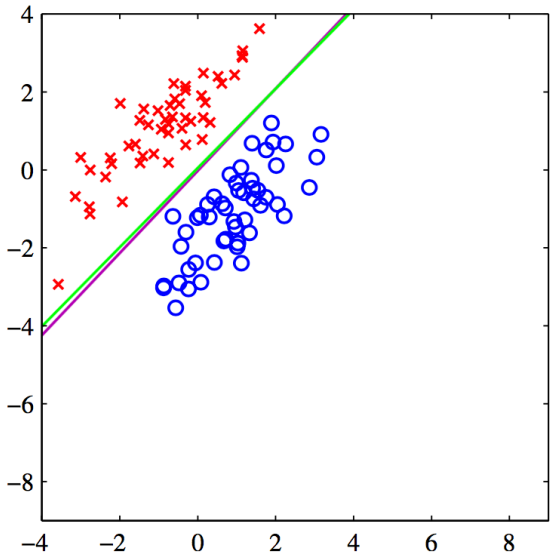
  - Boundary is perpendicular to weight vector $\mathbf{w}$

[Bishop]

- Classifier Score($\mathbf{x}_i$) = $h(\mathbf{x}_i; \mathbf{w})$

- Class predictions: Predict class 0 if $h(\mathbf{x}_i ; \mathbf{w}) < 0$, else class 1

Linear Classifier with Least Squares?

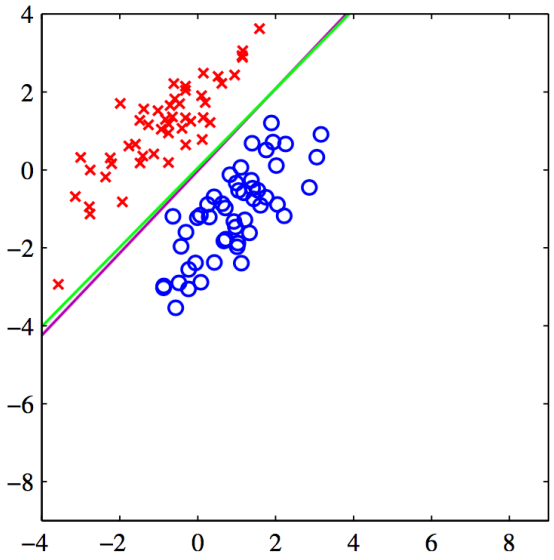


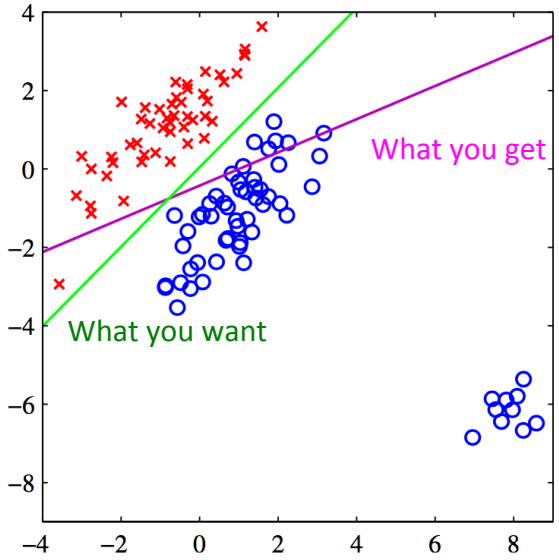
$$L(\mathbf{w}) = \frac{1}{2}\sum_i (y_i - \mathbf{w}^T\mathbf{x}_i)^2$$

[Bishop]

- Why not use least squares loss with binary targets?

Linear Classifier with Least Squares?





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[Bishop]

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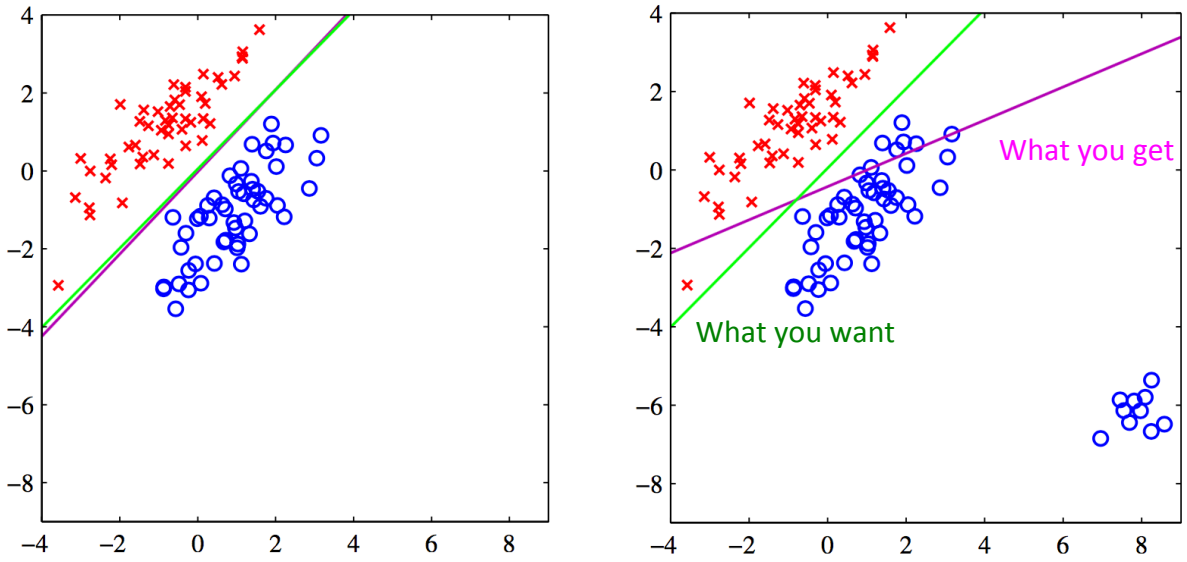
  - Penalized even when predict class correctly
  - Least squares is very sensitive to outliers

Linear Classifier with Least Squares?



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[Bishop]

- Why not use least squares loss with binary targets?
  - Penalized even when predict class correctly
  - Least squares is very sensitive to outliers
- Use only class labels?
  - Perceptron algorithm (not covered here)
- A probabilistic approach?

Logistic Regression for Classification

- Set of input / output pairs $D = \{\mathbf{x}_i , y_i\}_{i=1\ldots n}$
  - $\mathbf{x}_i \in \mathbb{R}^m$
  - $y_i \in \{0, 1\}$

- Linear discriminant: $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T\mathbf{x}$

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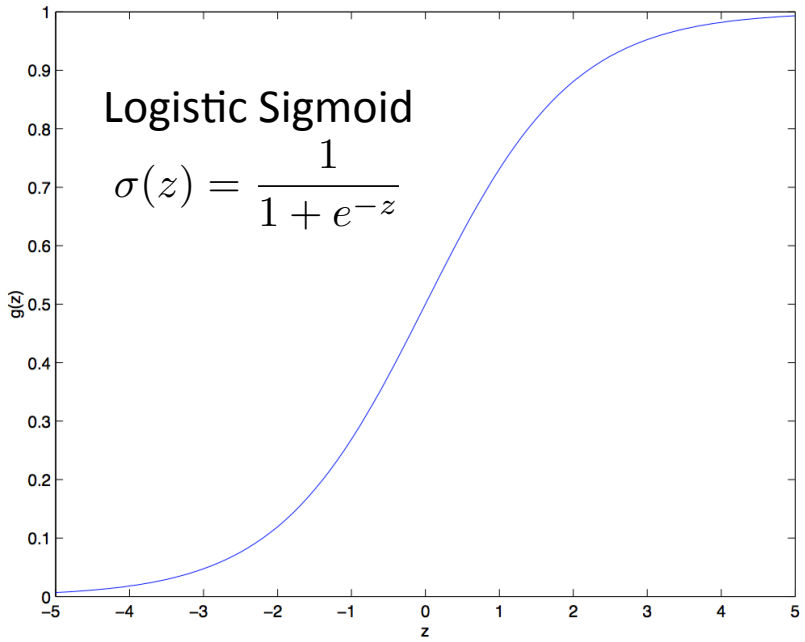
- Model per example probability: $p(y = 1|\mathbf{x}) \equiv p_i = \dfrac{1}{1 + e^{-h(\mathbf{x};\mathbf{w})}}$

$$= \frac{1}{1 + e^{-\mathbf{w}^T\mathbf{x}}}$$



NOTE:
Not a random choice,
Natural choice for large class of models

See backups for more info

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- Concisely write $p(y|\mathbf{x})$ as Bernoulli random variable:

$$P(y_i = y|x_i) = \text{Bernoulli}(p_i) = (p_i)^{y_i}(1 - p_i)^{1-y_i} = \begin{cases} p_i & \text{if } y_i=1 \\ 1\text{-}p_i & \text{if } y_i=0 \end{cases}$$

Logistic Regression

- Negative log-likelihood

$$-\ln \mathcal{L} = -\ln \prod_i (p_i)^{y_i} (1-p_i)^{1-y_i}$$

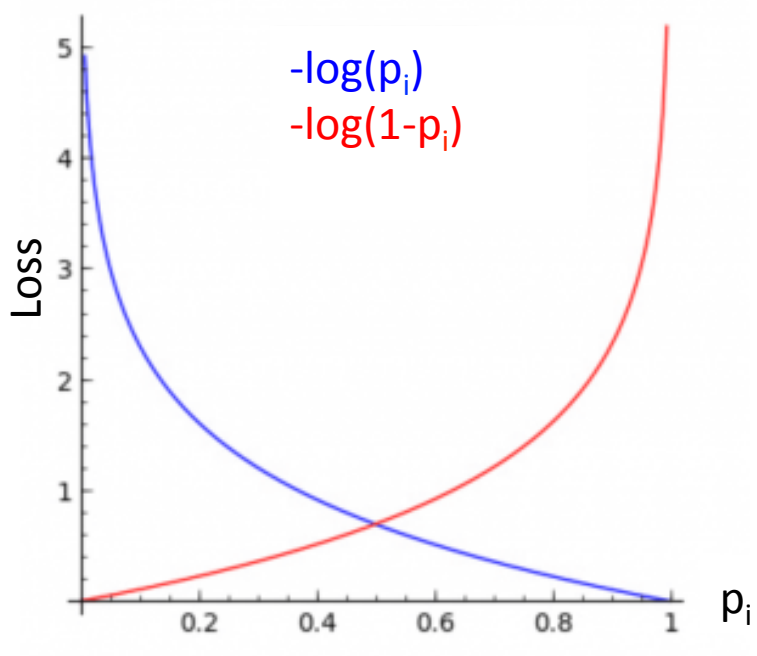
Logistic Regression

- Negative log-likelihood

$$-\ln \mathcal{L} = -\ln \prod_i (p_i)^{y_i} (1-p_i)^{1-y_i}$$

$$= -\sum_i y_i \ln(p_i) + (1-y_i) \ln(1-p_i)$$

binary cross entropy loss function!



Logistic Regression

- Negative log-likelihood

$$-\ln \mathcal{L} = -\ln \prod_i (p_i)^{y_i} (1-p_i)^{1-y_i}$$

$$= -\sum_i y_i \ln(p_i) + (1-y_i) \ln(1-p_i)$$

$$= \sum_i y_i \ln(1+e^{-\mathbf{w}^T\mathbf{x}}) + (1-y_i) \ln(1+e^{\mathbf{w}^T\mathbf{x}})$$

binary cross entropy loss function!

- No closed form solution to $\mathbf{w}^* = \arg\min_{\mathbf{w}}$ -ln L
- How to solve for **w**?

Gradient Descent

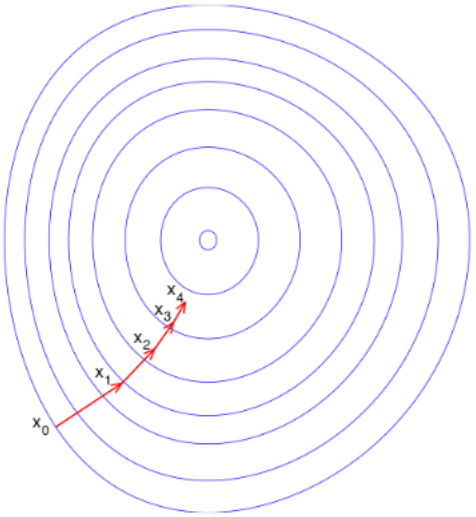
- Many methods to solve, lets us **Gradient Descent**

- Minimize loss by repeated gradient steps (when no closed form)

  - Compute gradient w.r.t. parameters: $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$

  - Update parameters $\mathbf{w}' \leftarrow \mathbf{w} - \eta \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$

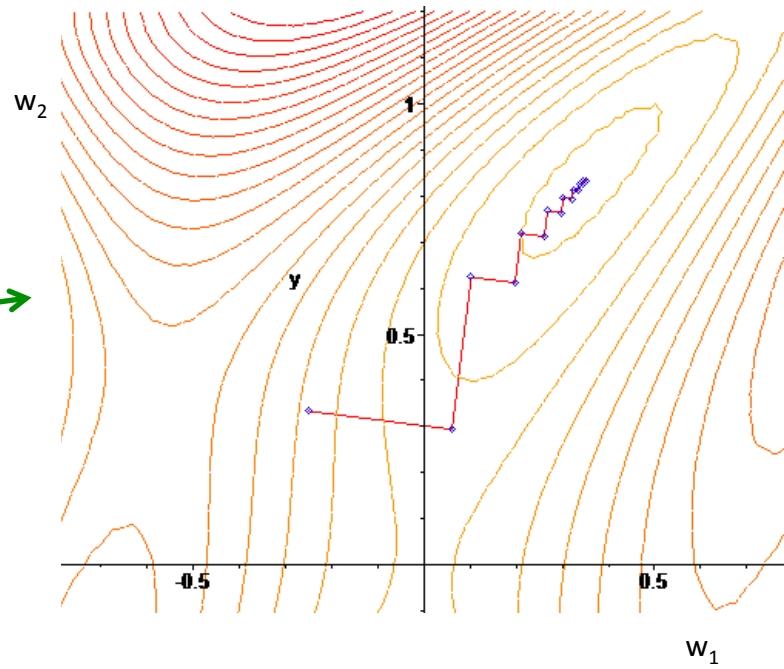
  - η is called the learning rate, controls how big of a gradient step to take

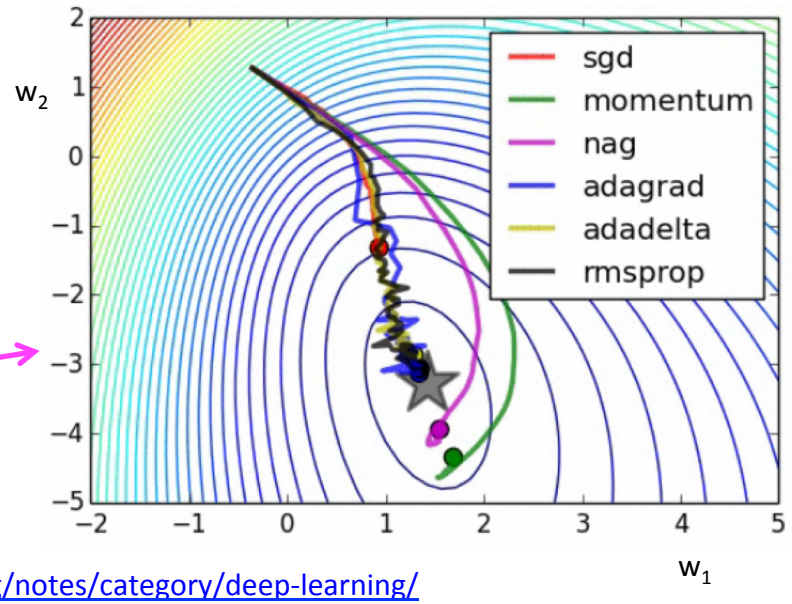


Stochastic Gradient Descent and Variants

- Gradient descent is computationally costly (since we compute gradient over full training set)

- Stochastic gradient descent
  - Compute gradient on one event at a time (in practice a small batch)
  - Noisy estimates average out
  - Stochastic behavior can allow "jumping" out of bad critical points
  - Scales well with dataset and model size
  - But can have some convergence difficulties
  - Improvements include: Momentum, RMSprop, AdaGrad, …





http://danielnouri.org/notes/category/deep-learning/

Gradient Descent for Logistic Regression

$$L(\mathbf{w}) = -\ln \mathcal{L}(\mathbf{w}) = -\sum_i y_i \ln(\sigma(\mathbf{w}^T\mathbf{x})) + (1-y_i)\ln(1-\sigma(\mathbf{w}^T\mathbf{x}))$$

- Derivative of sigmoid: $\frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1-\sigma(z))$

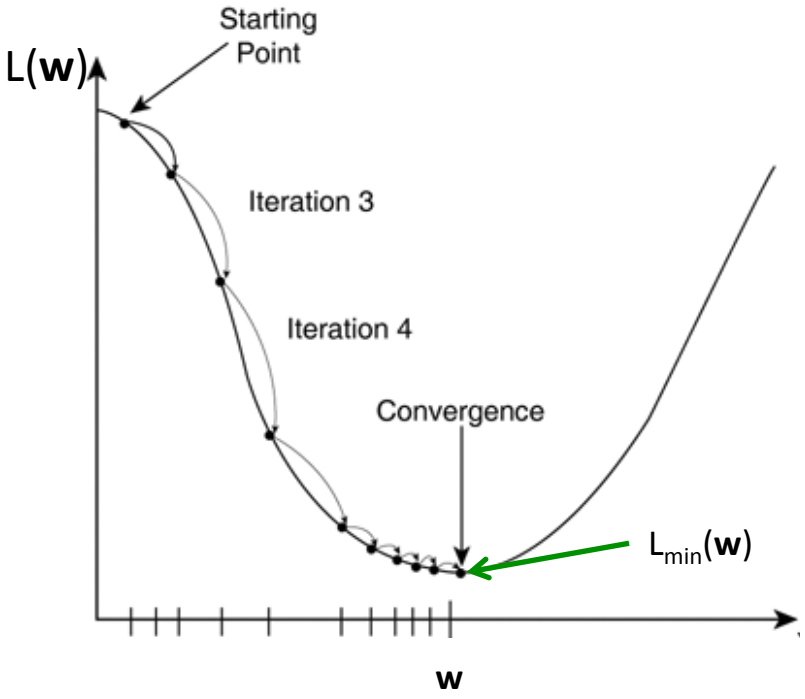
- Derivative of Loss: $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \sum_i (\sigma(\mathbf{w}^T\mathbf{x}) - y_i)\mathbf{x}_i$

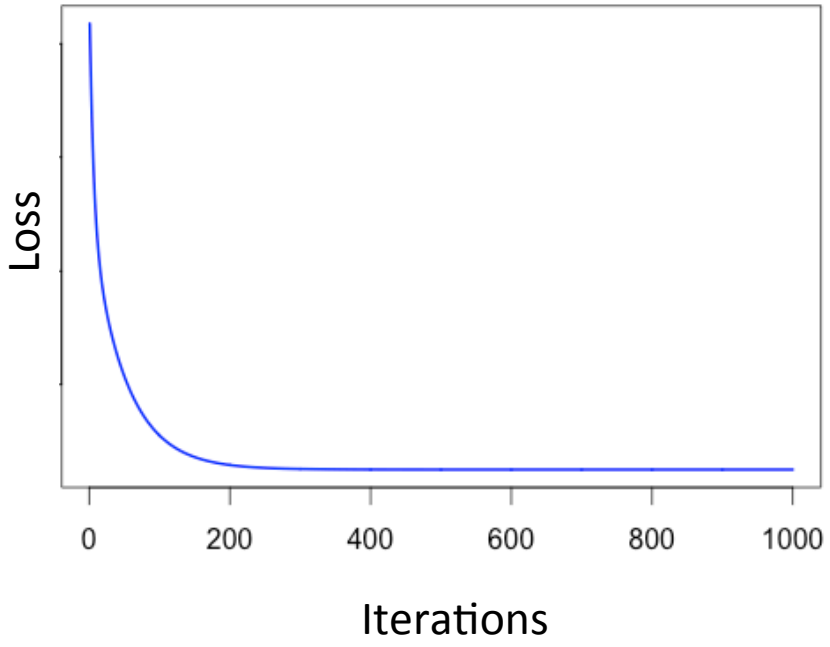
- Update rule:

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}} = \mathbf{w} - \eta \sum_i (\sigma(\mathbf{w}^T\mathbf{x}) - y_i)\mathbf{x}_i$$

- Repeat until parameters stable

Gradient Descent

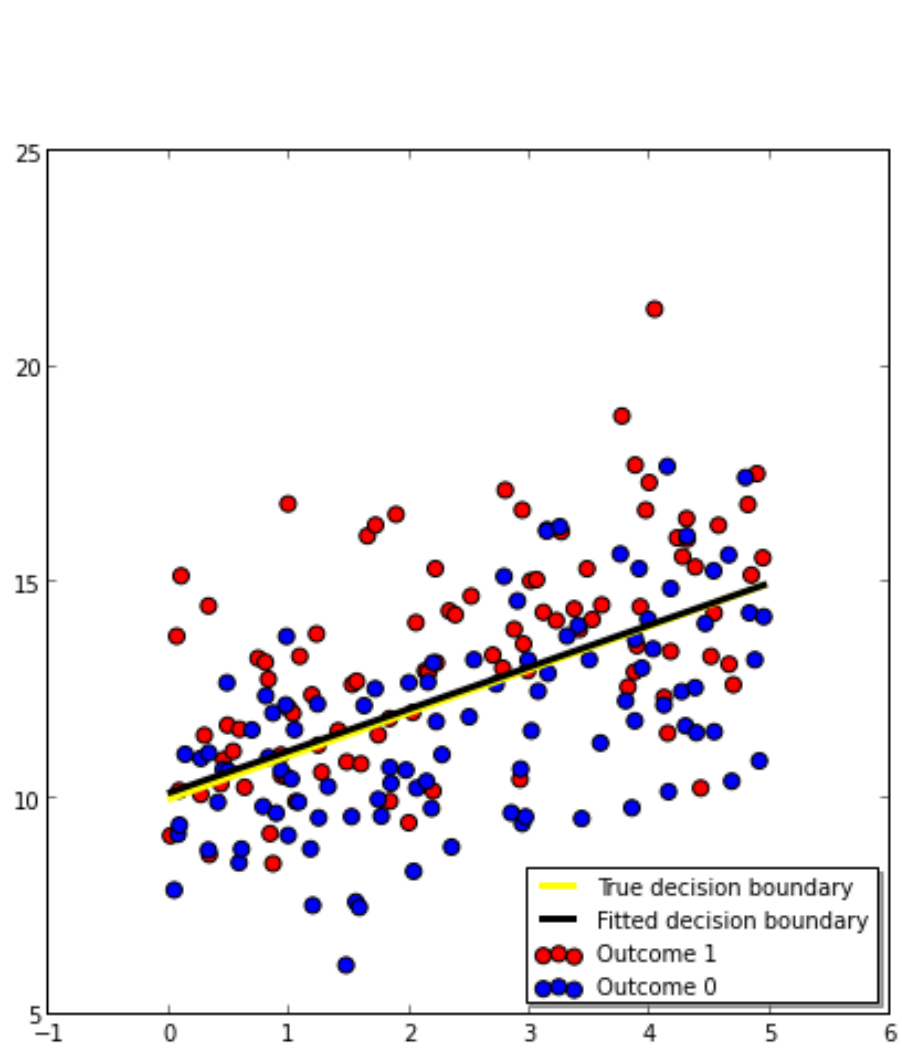


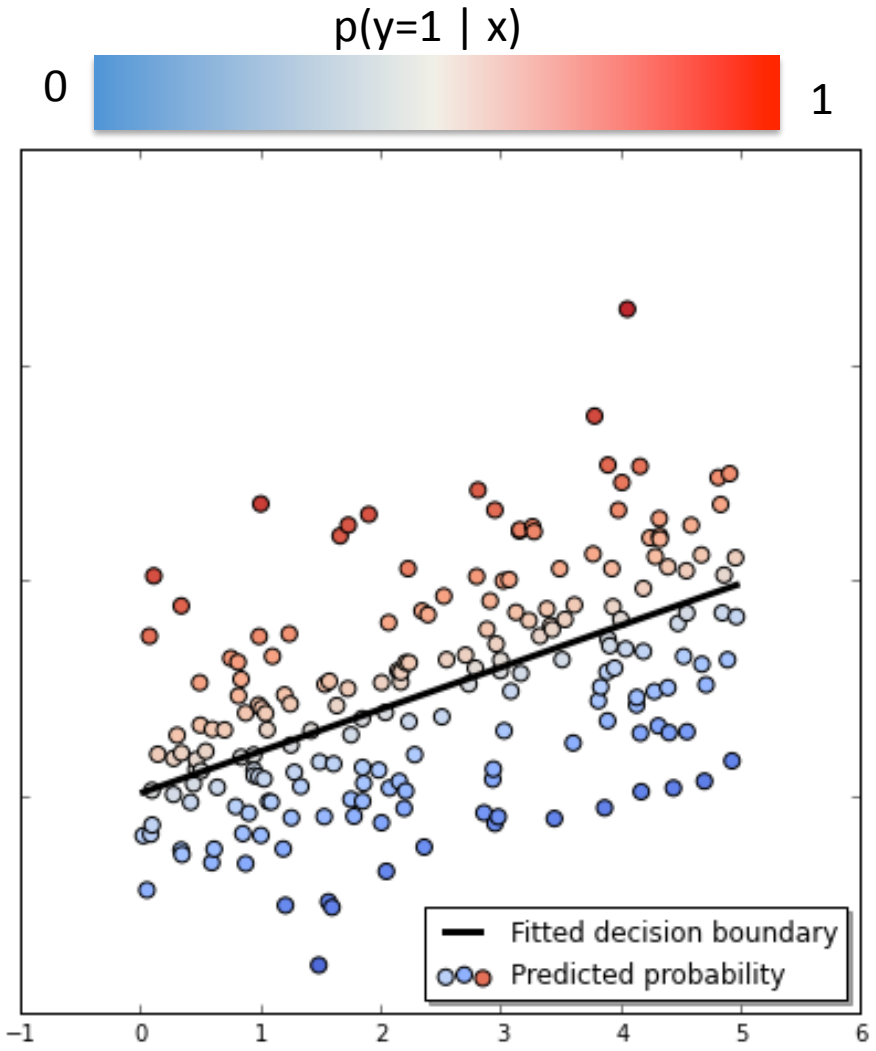


- Loss is convex
  - Single global minimum

- Iterations lower loss and move toward minimum

Logistic Regression Example



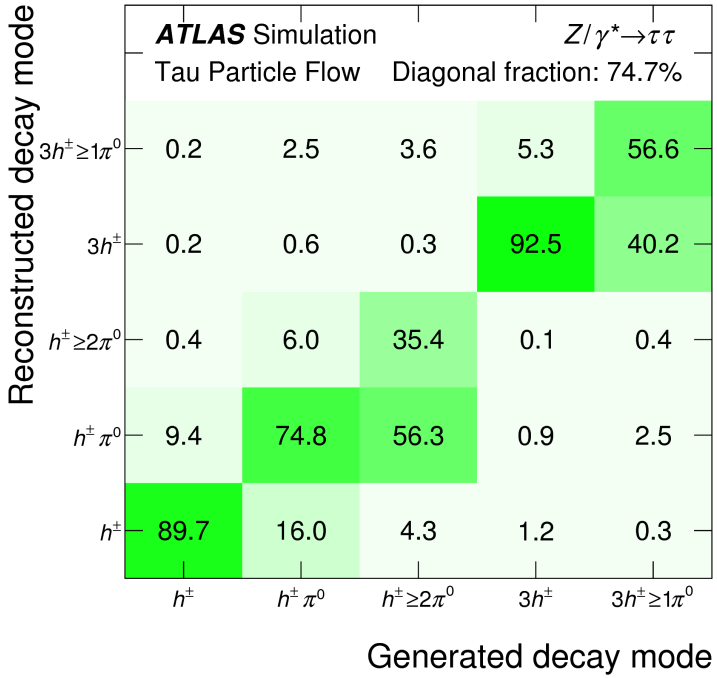


https://triangleinequality.wordpress.com/2013/12/02/logistic-regression/

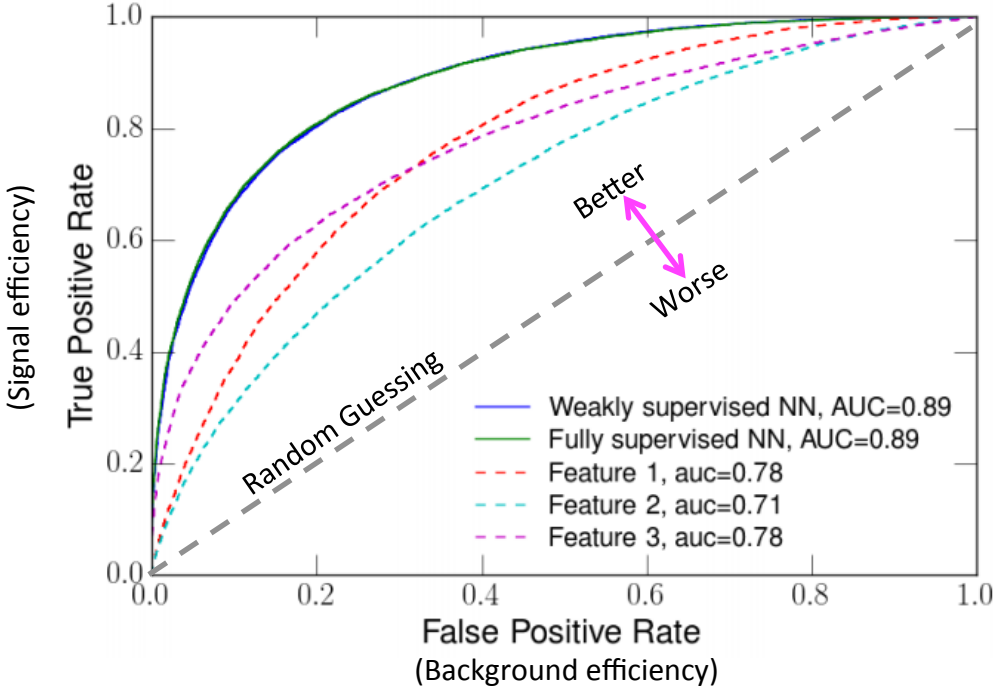
Estimating a Classifier Performance

		Predicted: Positive	Predicted: Negative
True	Positive	True Positives (TP)	False Negatives (FN)
True	Negative	False Positives (FP)	True Negatives (TN)

Confusion Matrix
Classifying tau decays



Receiver Operating Characteristic (ROC) Curve
classifying quarks vs. gluons

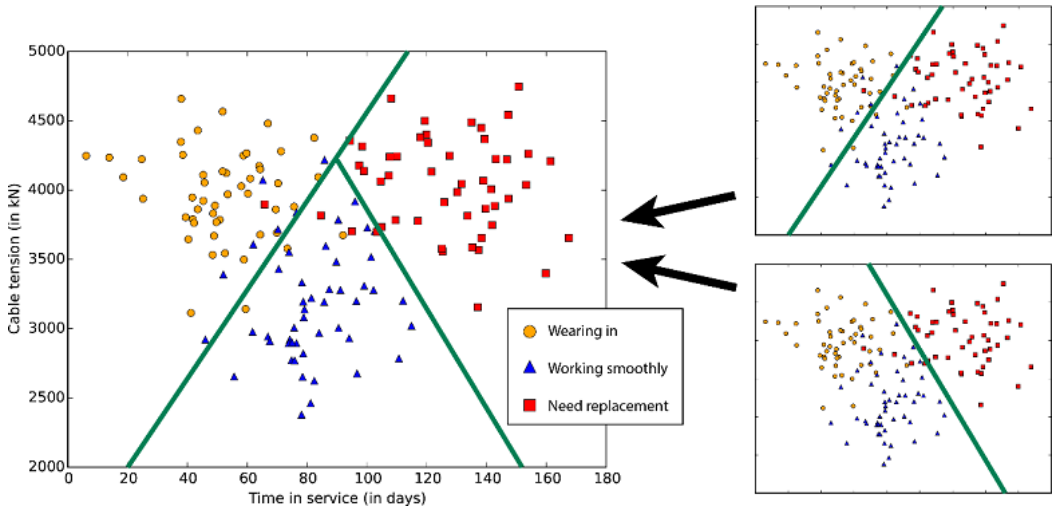


arXiv:1512.05955

arXiv:1702.00414

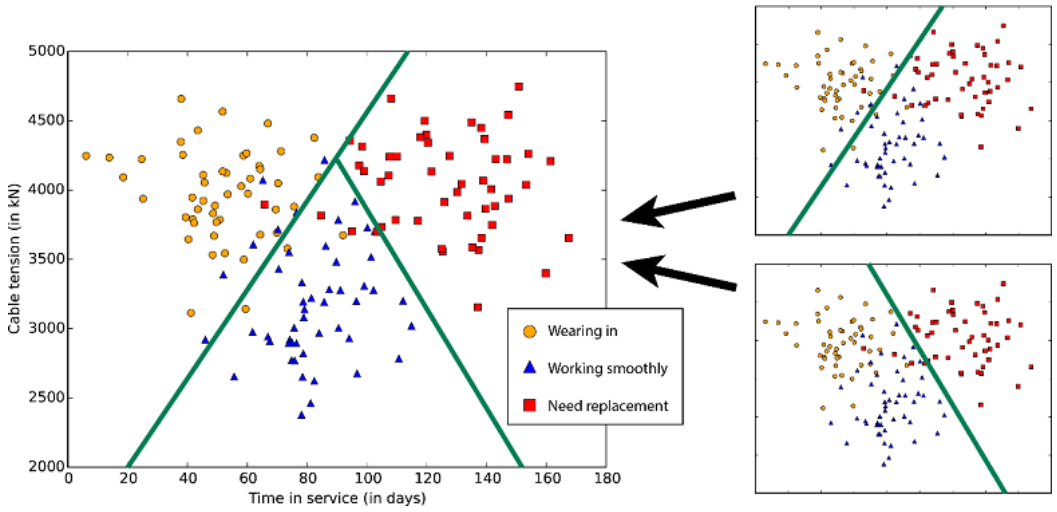
Multiclass Classification?

- What if there is more than two classes?



Multiclass Classification?

- What if there is more than two classes?



- Softmax → multi-class generalization of logistic loss
  - Have N classes $\{c_1, \ldots, c_N\}$
  - Model target $\mathbf{y}_k = (0, \ldots, 1, \ldots 0)$

k^{th} element in vector

$$p(c_k|x) = \frac{\exp(\mathbf{w}_k x)}{\sum_j \exp(\mathbf{w}_j x)}$$

  - Gradient descent for each of the weights $\mathbf{w}_k$

Summary of Today

- Machine learning uses mathematical and statistical models learned from data to characterize patterns and relations between inputs, and use this for inference / prediction

- Machine learning comes in many forms, much of which has probabilistic and statistical foundations and interpretations (i.e. *Statistical Machine Learning*)

- Discussed linear models today
  - Many forms of linear models, we only touched the surface!

- Next time, some nonlinear models and unsupervised learning
  - Decision trees and ensemble methods
  - Neural network (intro)
  - Clustering
  - Dimensionality reduction

Advertisements

- Friday's lecture on deep learning and computer vision from John Shlen from Google Brain!

- Data Science @ HEP workshop on machine learning in high energy physics
  - May 8-12, 2017 at Fermilab
  - https://indico.fnal.gov/conferenceDisplay.py?ovw=True&confId=13497

Recommended Materials

- Many excellent books (many available free online)
  - Introduction to Statistical Learning
  - Elements of Statistical Learning
  - Pattern Recognition and Machine learning (Bishop)
  - …
- Many excellent courses and documentation available online
  - Andre Ng's machine learning course on Coursera
  - University course material online: Stanford CS229, Harvard CS181, …
  - Lectures from Machine Learning Summer School (MLSS)
  - Lectures from Yandex Machine learning in HEP summer schools
  - Scikit Learn documentation
  - …
- **References**:
  - I used / borrowed from many of these references to make these lectures!

References

- http://scikit-learn.org/
- [Bishop] Pattern Recognition and Machine Learning, Bishop (2006)
- [ESL] Elements of Statistical Learning (2nd Ed.) Hastie, Tibshirani & Friedman 2009
- [Murray] Introduction to machine learning, Murray
  - http://videolectures.net/bootcamp2010_murray_iml/
- [Ravikumar] What is Machine Learning, Ravikumar and Stone
  - http://www.cs.utexas.edu/sites/default/files/legacy_files/research/documents/MLSS-Intro.pdf
- [Parkes] CS181, Parkes and Rush, Harvard University
  - http://cs181.fas.harvard.edu
- [Ng] CS229, Ng, Stanford University
  - http://cs229.stanford.edu/
- [Rogozhnikov] Machine learning in high energy physics, Alex Rogozhnikov
  - https://indico.cern.ch/event/497368/

Bayesian vs. Frequentist Models

- Mathematical models in ML typically described via random variables — in which case they are also called statistical models
- Statistical models typically specified by **unknown** parameters (to be learnt from data)
- **Frequentist:** there exist a "ground-truth" set of unknown parameters that are constant (i.e. not random)
- **Bayesian:** model parameters are themselves random, and typically specified by their own distribution/statistical model, with their own unknown "hyperparameters"

Probabilistic Motivation

- Posterior probability: $p(y=1|\mathbf{x}) = \frac{p(\mathbf{x}|y=1)p(y=1)}{p(\mathbf{x}|y=1)p(y=1)+p(\mathbf{x}|y=0)p(y=0)}$

$$= \frac{1}{1+e^{-a(\mathbf{x})}} = \sigma(a(\mathbf{x}))$$

Logistic sigmoid

- Log-probability ratio: $a(\mathbf{x}) = \ln \frac{p(\mathbf{x}|y=1)p(y=1)}{p(\mathbf{x}|y=0)p(y=0)}$

- In a large class of models $a(\mathbf{x})$ is linear

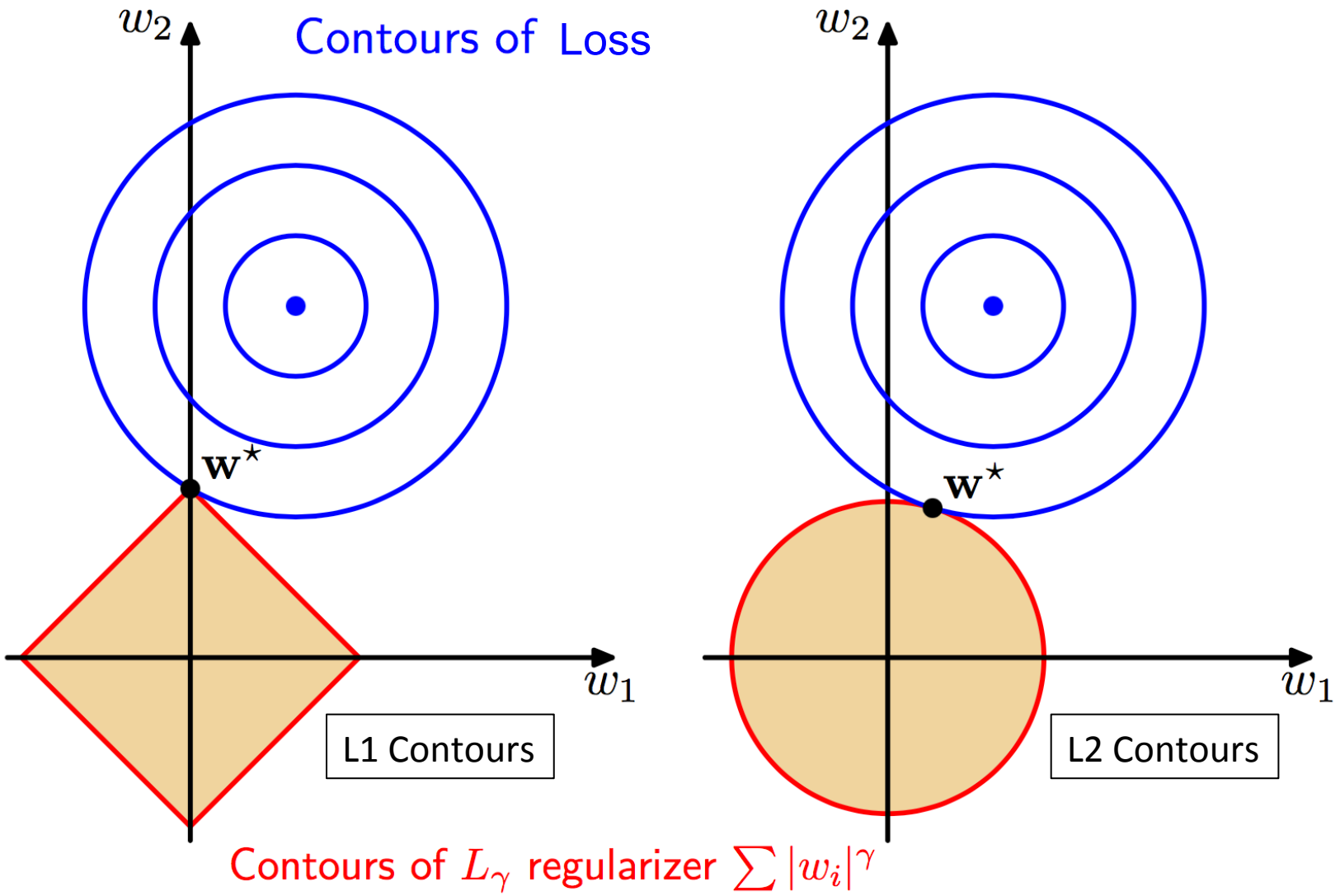
$$a(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$$

  - When class-conditional density $p(\mathbf{x}|y)$ is in the exponential family of Generalized Linear Models,
    - Includes Gaussian, Exponential, Poisson, Beta, …

- Have linear discriminant and estimate of per-class probability

- Even if $p(\mathbf{x}|y)$ unknown, motivation to model $p(y|\mathbf{x})$ with logistic sigmoid

Regularization



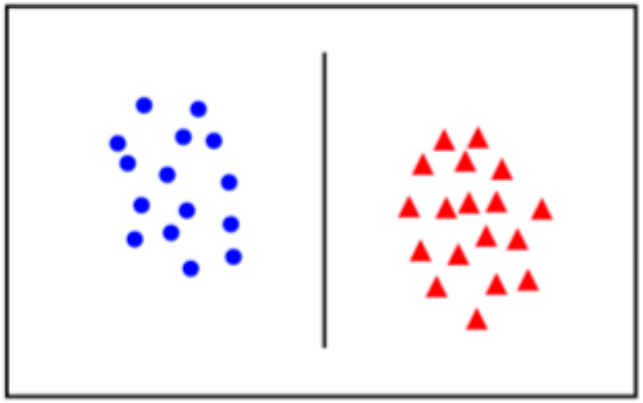
Contours of L_γ regularizer $\sum |w_i|^\gamma$

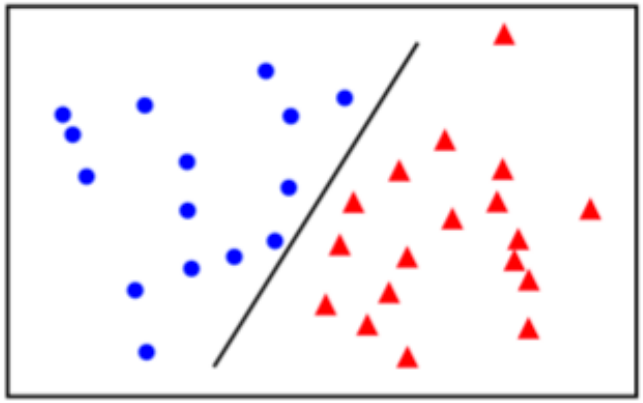
Pattern Recognition and Machine Learning C. M. Bishop (2006)

Support Vector Machines

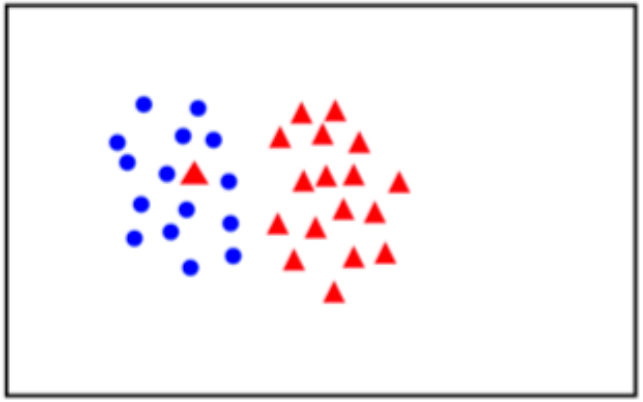
Linear Separability

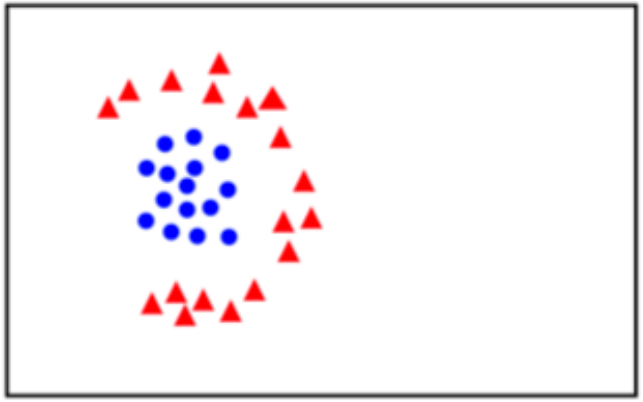
linearly separable



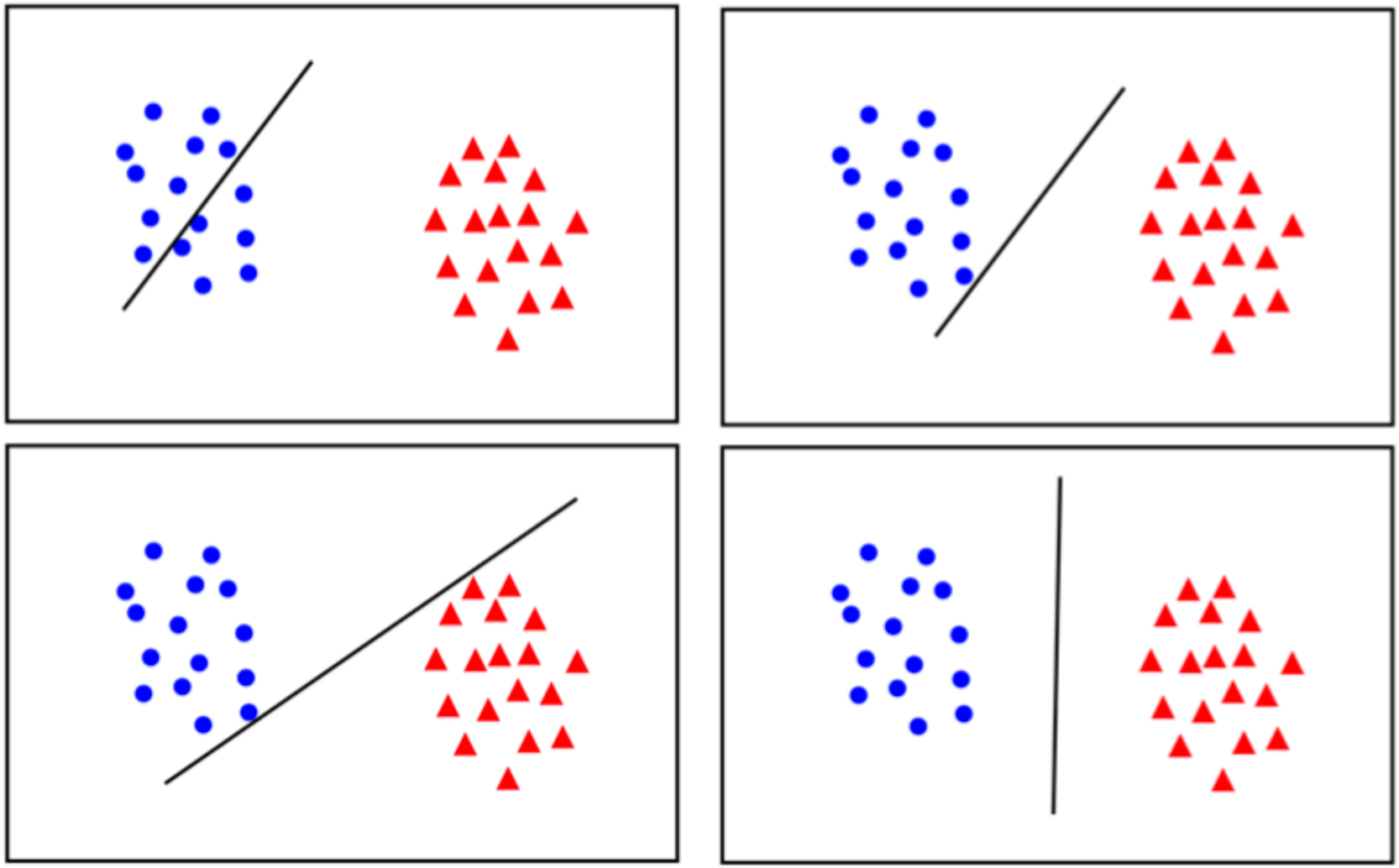


not linearly separable





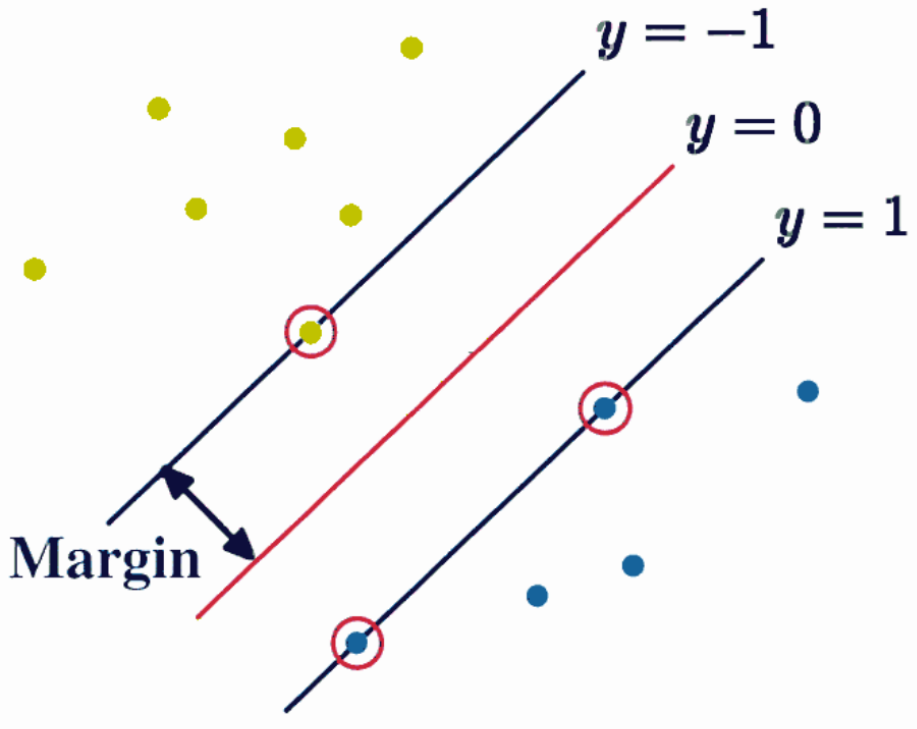
Decision Boundaries – Which is Best?



Maximum Margin Classifiers

- Many possible solutions to separating classes
  - Depends on the loss function chosen

- Assuming classes are linearly separable, what if we wanted to solution with the maximum distance between the decision boundary and the nearest data point?



Maximum Margin Classifier

- Assume we have:
  - x in R^d
  - y in {-1, 1}

- Linear classifier: $h(\mathbf{x}; \mathbf{w}) = \mathbf{w}^T\mathbf{x} + w_0$

- Distance of data point, $\mathbf{x}_i$, to decision boundary $\dfrac{y_i(\mathbf{w}^T\mathbf{x}_i + w_0)}{\sqrt{\mathbf{w}^T\mathbf{w}}}$

- Optimization problem:

$$\arg\max_{\mathbf{w},\ w_0} \left\{ \frac{1}{\sqrt{\mathbf{w}^T\mathbf{w}}} \min_i y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \right\} \longrightarrow \arg\min_{\mathbf{w}, w_0} \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$$s.\ t.\ \ y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 \text{ for all } i$$

  - Can solve with gradient descent methods!

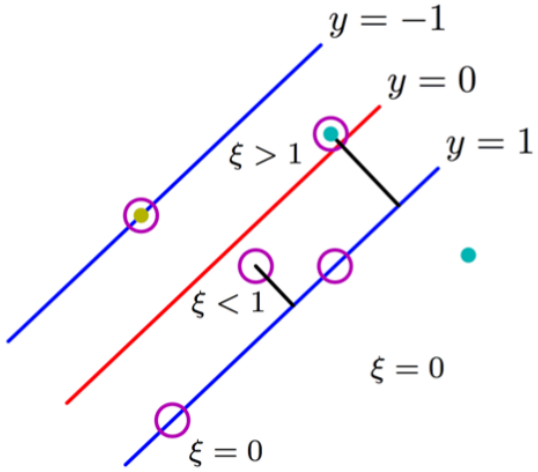
What if points not linearly separable?

$$\arg\min_{\mathbf{w},w_0} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_i \xi_i$$

$$s.\,t.\;\; y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi_i \text{ for all } i$$

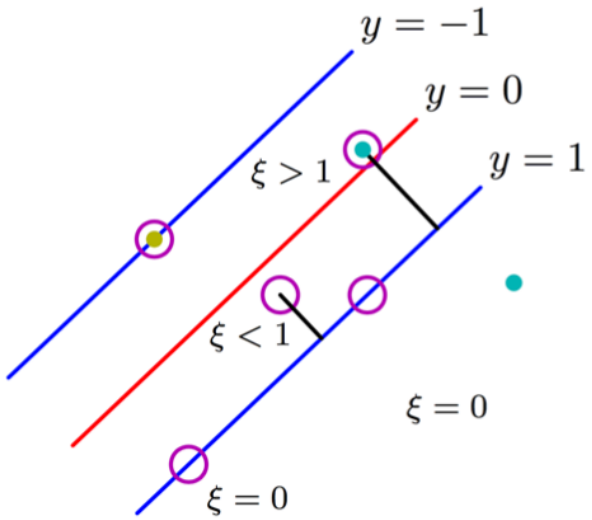
$$\text{and } \xi_i \geq 0$$

- Add a smearing to the margin, $\xi \geq 0$
  - If $\xi = 0$, example correctly classifier
  - If $0 < \xi < 1$, example correctly classified, but in margin
  - If $\xi > 1$, example incorrectly classified



- Add regularizer to problem to constrain ξ_i not too large
  - C is the regularization hyperparameter that controls how much "softening" of the boundary is allowed, thus how big is margin

What if points not linearly separable?

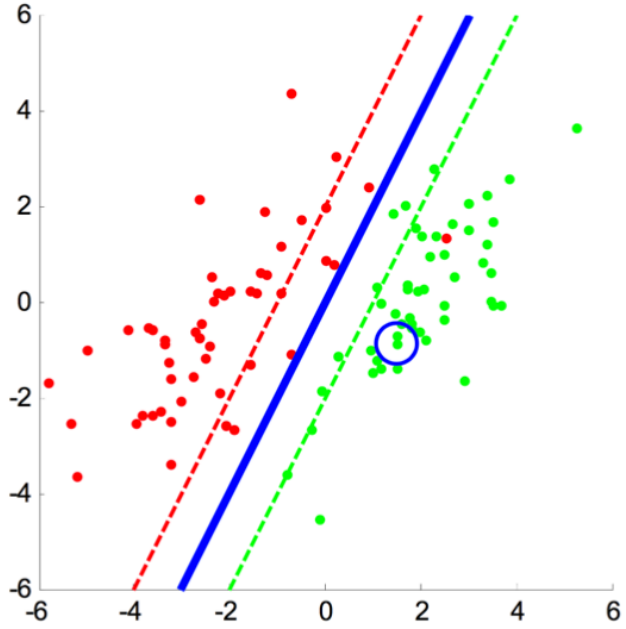


$$\arg\min_{\mathbf{w},w_0} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_i \xi_i$$

$$s.\,t.\quad y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi_i \text{ for all } i$$

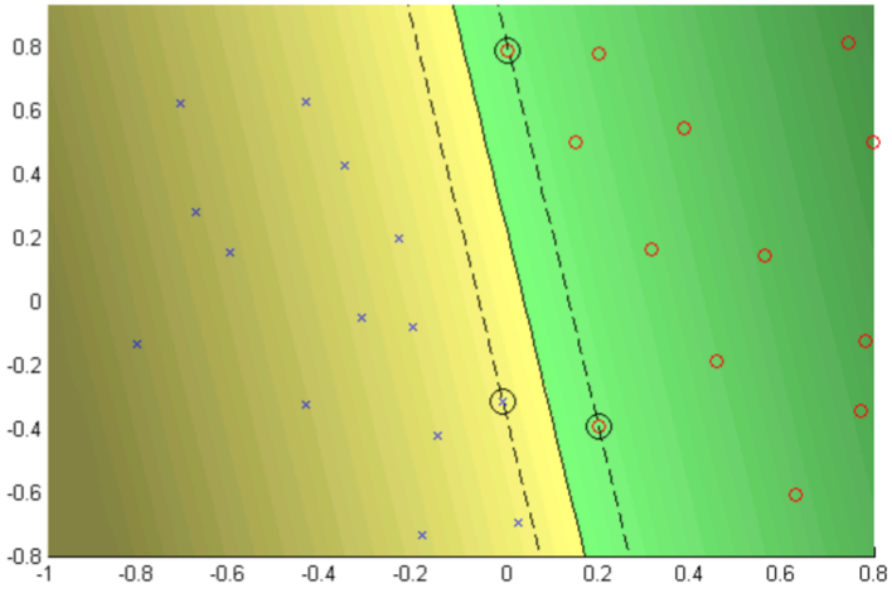
$$\text{and}\quad \xi_i \geq 0$$

- Add a smearing to the margin, $\xi \geq 0$
- Add regularizer to problem to constrain ξ_i not too large
- C is the regularization hyperparameter
  - Controls how much "softening" of the boundary is allowed, thus how big is margin

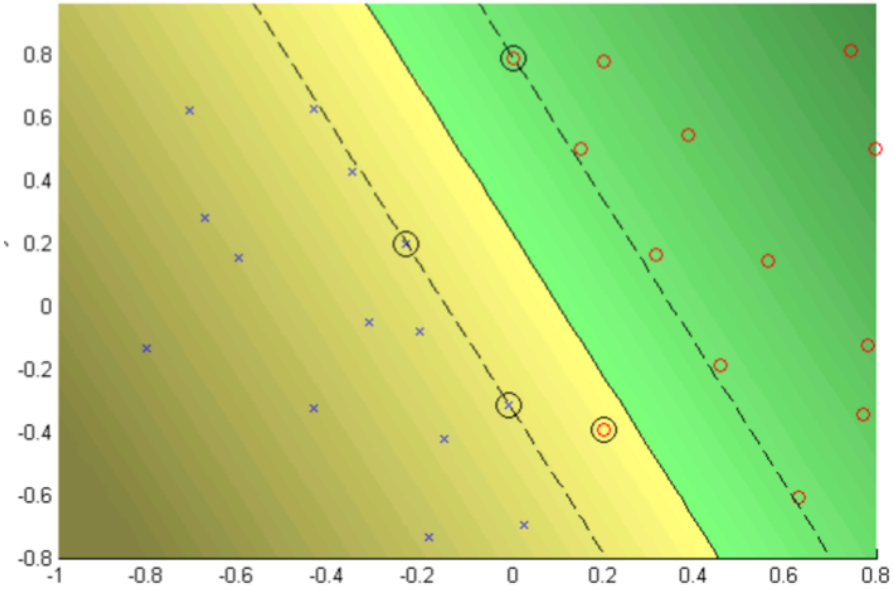


Soft Margin Formulation

C=infinity, hard margin



C=10, soft margin



Dual Formulation

- Use Lagrange multipliers (remember those!) to write a loss function for hard margin:

$$L(\mathbf{w}, w_0, \mathbf{a}) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_i a_i\{y_i(\mathbf{w}^T\mathbf{x}_i + w_0) - 1\}$$

$$s.\ t.\ \ \{a_i \geq 0\}$$

  - Where **a** are Lagrange multipliers
  - Minimize L w.r.t. **w** and w_0:

$$\rightarrow \mathbf{w} = \sum_i a_i y_i x_i$$

$$\rightarrow \sum_i a_i y_i = 0$$

- Dual form of optimization
  - Solve for **a** and w_0 using gradient methods, or SMO algorithm

$$\max_{\mathbf{a}} \sum_i a_i - \frac{1}{2}\sum_i\sum_j a_i a_j y_i y_j \mathbf{x}_i^t \mathbf{x}_j$$

$$s.\ t.\ \sum_i a_i y_i = 0$$

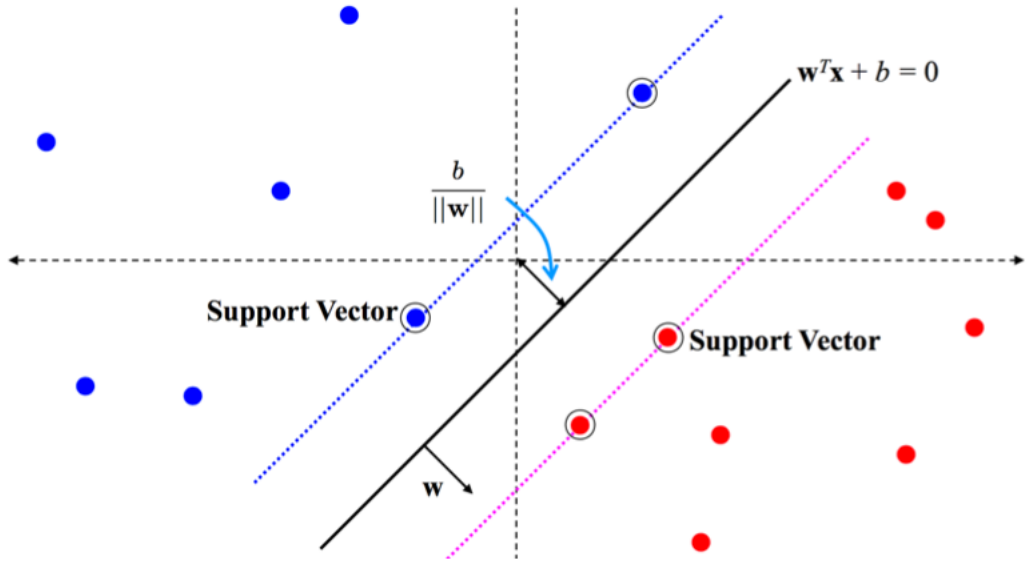
$$a_i \geq 0 \text{ for all } i$$

Discriminant Function

$$h(\mathbf{x}; \mathbf{a}, w_0) = \sum_i a_i y_i \mathbf{x}_i^t \mathbf{x} + w_0$$

Support Vector Machines

$$h(\mathbf{x}; \mathbf{a}, w_0) = \sum_i a_i y_i \mathbf{x}_i^t \mathbf{x} + w_0$$



- Only examples on margin will have $a_i > 0$!
  - Follows from KKT conditions of constrained optimization
- Sum is only over a small number of examples on margin, the **support vectors**
  - Note: also only depends on inner produce! More later
- Margin on data = $1/||\mathbf{w}||$
  - At least one constraint will hold

Support Vector Machines: Recap

- Maximum Margin Optimization: $\max_{\mathbf{a}} \sum_i a_i - \frac{1}{2} \sum_i \sum_j a_i a_j y_i y_j \mathbf{x}_i^t \mathbf{x}_j$
  - Dual formulation

$$s.\ t.\ \sum_i a_i y_i = 0$$

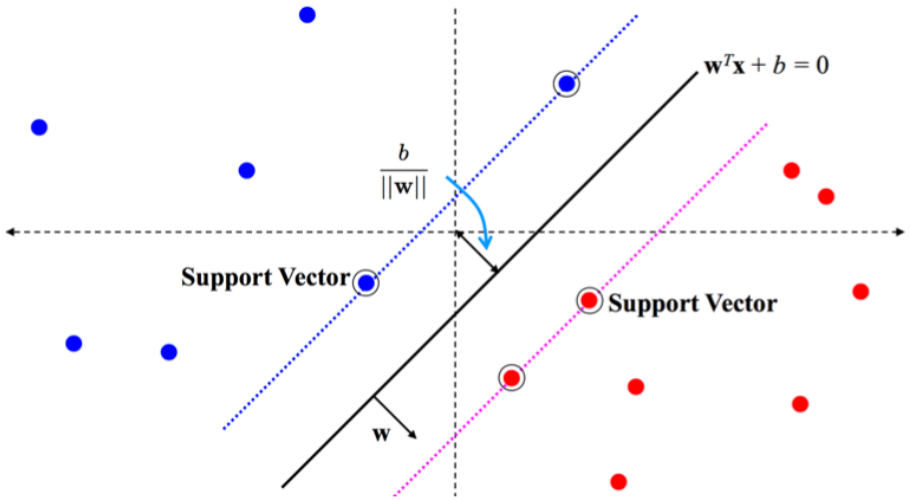
$$a_i \geq 0 \text{ for all } i$$

Data always in inner product

- Discriminant function:

$$h(\mathbf{x}; \mathbf{a}, w_0) = \sum_i a_i y_i \mathbf{x}_i^t \mathbf{x} + w_0$$

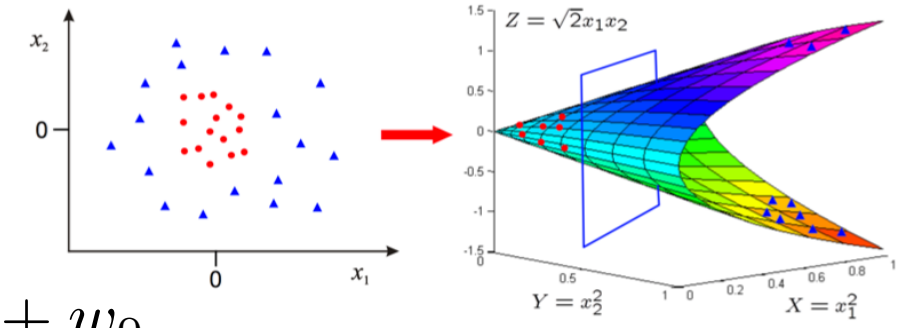
  - Sum is only over a small number of examples on margin called the **support vectors**



Basis Functions Revisited

- When data is not linearly separable, can use basis functions

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \quad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$



$$h(\mathbf{x}; \mathbf{a}, w_0) = \sum_i a_i y_i \phi(\mathbf{x}_i)^T \phi(\mathbf{x}) + w_0$$

- Where ϕ is a map from $R^m \rightarrow R^k$
- But if k>>>m (or if k infinite), inner product can be expensive to compute
- But we don't need the mapping ϕ, only inner products…

Kernels and the Kernel Trick

- A kernel function K(x,x')=ϕ(x)ϕ(x') is an inner product where ϕ is a mapping $R^m \rightarrow R^k$

- Kernelized discriminant and optimization problem

$$h(\mathbf{x}; \mathbf{a}, w_0) = \sum_i a_i y_i K(\mathbf{x}_i, \mathbf{x}) + w_0$$

$$\max_{\mathbf{a}} \sum_i a_i - \frac{1}{2} \sum_i \sum_j a_i a_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$s.\ t. \quad \sum_i a_i y_i = 0$$

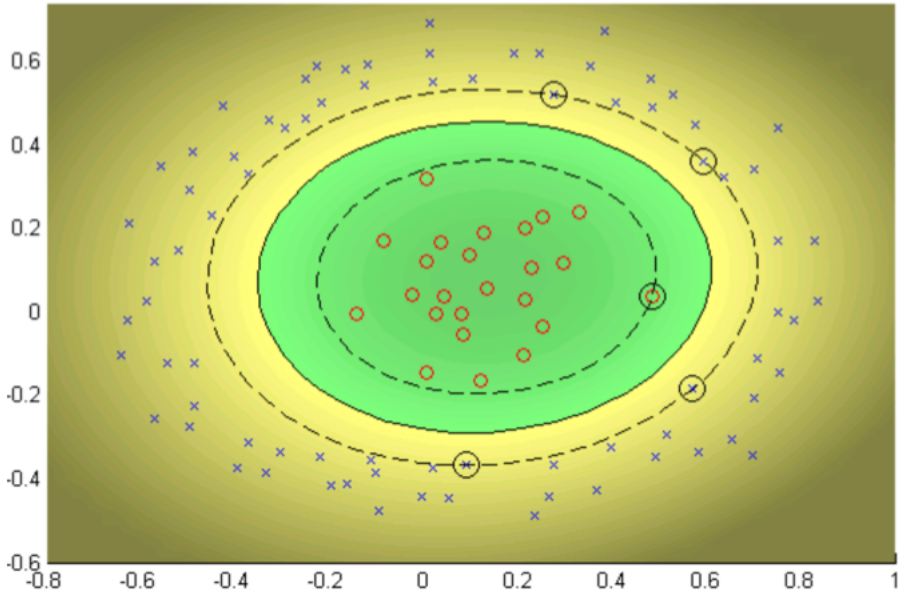
$$a_i \geq 0$$

- **Kernel Trick**: compute the Kernel K(x, x') without computing ϕ(x)!
  - So we just need to engineer the Kernel, not the exact features or exact mapping

Kernels

- Linear Kernel: $K(\mathbf{x},\mathbf{x}') = \mathbf{x}^T\mathbf{x}'$
- Polynomial Kernel: $K(\mathbf{x},\mathbf{x}') = (1 + \mathbf{x}^T\mathbf{x}')^q$
- Gaussian Kernal: $K(\mathbf{x},\mathbf{x}') = \exp\left(-\frac{1}{2}\frac{(\mathbf{x}-\mathbf{x}')^2}{\sigma^2}\right)$
- As long as the Kernel matrix $K_{ij} = \phi(\mathbf{x}_i)\,\phi(\mathbf{x}_j)$ is a positive semi-definite matrix, it is a valid Kernel

Gaussian Kernel with σ=1



Gaussian Kernel with σ=0.25