

General

Dataset and Definitions

\mathcal{D} is a set of training examples, the n -th Training Example ($n = 1, 2, \dots, N$), of this set is:

$$\mathbf{x}_n = [x_{n1} \ x_{n2} \ \dots \ x_{nD}]^T$$

We write all N training examples in a matrix:

$$\mathbf{X} = [\mathbf{x}_1^T; \mathbf{x}_2^T; \dots; \mathbf{x}_N^T]$$

In supervised learning, you are also given a set of observations corresponding to the training examples:

$$\mathbf{y} = [y_1 \ y_2 \ \dots \ y_N]^T$$

We assume a *true* model behind the data, the observations are noisy versions of this ground truth:

$$y = y_{true} + \epsilon.$$

The final goal is to predict a $\hat{y} = f(\hat{\mathbf{x}})$ given any $\hat{\mathbf{x}}$.

Eigendecomposition: \mathbf{A} diagonalizable $N \times N$ matrix with N linearly independent eigenvectors, q_i , can be factorized as $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}$ where \mathbf{Q} is square ($N \times N$) and has its i th column equal the eigenvector q_i of \mathbf{A} and $\mathbf{\Lambda}$ is the diagonal matrix with $\Lambda_{ii} = \lambda_i$.

Vector and matrix derivatives

First Order

$$\frac{\partial \mathbf{x}^T \mathbf{a}}{\partial \mathbf{x}} = \frac{\partial \mathbf{a}^T \mathbf{x}}{\partial \mathbf{x}} = \mathbf{a} \quad \frac{\partial \mathbf{a}^T \mathbf{X} \mathbf{b}}{\partial \mathbf{X}} = \mathbf{a} \mathbf{b}^T$$

$$\frac{\partial \mathbf{a}^T \mathbf{X}^T \mathbf{b}}{\partial \mathbf{X}} = \mathbf{b} \mathbf{a}^T \quad \frac{\partial \mathbf{a}^T \mathbf{X} \mathbf{a}}{\partial \mathbf{X}} = \frac{\partial \mathbf{a}^T \mathbf{X}^T \mathbf{a}}{\partial \mathbf{X}} = \mathbf{a} \mathbf{a}^T$$

Second Order

$$\frac{\partial \mathbf{b}^T \mathbf{X}^T \mathbf{X} \mathbf{c}}{\partial \mathbf{X}} = \mathbf{X}(\mathbf{b} \mathbf{c}^T + \mathbf{c} \mathbf{b}^T)$$

$$\frac{\partial \mathbf{x}^T \mathbf{B} \mathbf{x}}{\partial \mathbf{x}} = (\mathbf{B} + \mathbf{B}^T) \mathbf{x}$$

$$\frac{\partial}{\partial \mathbf{A}} \log |\mathbf{A}| = \mathbf{A}^{-T}$$

Distributions

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

Multivariate gaussian distribution: $\mathcal{N}(\mathbf{X}|\mu, \Sigma)$

$$\Rightarrow p(\mathbf{X} = \mathbf{x}) =$$

$$(2\pi)^{-d/2} |\Sigma|^{-1/2} \exp[-\frac{1}{2}(\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu)]$$

Gaussian distribution: $\mathcal{N}(X|\mu, \sigma^2)$

$$\Rightarrow p(X = x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{1}{2}(\frac{x-\mu}{\sigma})^2)$$

Poisson distribution: $\mathcal{P}(X|\lambda)$

$$\Rightarrow p(X = k) = \frac{\lambda^k}{k!} \exp(-\lambda)$$

Binomial distribution: $f(k|n, p) = \binom{n}{k} p^k (1-p)^{n-k}$

Multinomial distribution:

$$f(x_1, \dots, x_k | n, \boldsymbol{\pi}) = \frac{n!}{x_1! \dots x_k!} \pi_1^{x_1} \dots \pi_k^{x_k}$$

Properties

A matrix \mathbf{M} is

positive (semi-)definite $\iff \forall$ nonzero vector \mathbf{a} , we have $\mathbf{a}^T \mathbf{M} \mathbf{a} > (=) 0$

symmetric $\mathbf{M}^T = \mathbf{M}$

singular if not invertible

invertible \iff full rank \iff p.d. \iff diag & diag $\neq 0 \iff \mathbf{M}^T$ invertible

$$(\mathbf{M}\mathbf{N})^T = \mathbf{N}^T \mathbf{M}^T$$

Jensen's inequality applied to log: If \mathbf{p} prob. distr.

and $t_k > 0$: $\log \sum_{k=1}^K p_k t_k \geq \sum_{k=1}^K p_k \log t_k$

Matrix inversion lemma:

$$(\mathbf{P}\mathbf{Q} + \mathbf{I}_N)^{-1} \mathbf{P} = \mathbf{P}(\mathbf{Q}\mathbf{P} + \mathbf{I}_M)^{-1}$$

Solution optimality of β^* :

$$1^{st}\text{-order necessary } \frac{\partial \mathcal{L}(\beta^*)}{\partial \beta} = 0$$

$$2^{nd}\text{-order sufficient } \mathbf{H}(\beta^*) := \frac{\partial^2 \mathcal{L}(\beta^*)}{\partial \beta \partial \beta^T} \text{ is p.s.d.}$$

Marginal and Conditional Gaussians:

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$$

$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1})$$

$$\Downarrow$$

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^T)$$

$$p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\Sigma}\{\mathbf{A}^T \mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\}, \boldsymbol{\Sigma})$$

$$\text{where } \boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \mathbf{A}^T \mathbf{L} \mathbf{A})^{-1}$$

Optimization methods

Grid Search $\mathcal{O}(M^D ND)$

Simply try M values for all parameters at regular intervals.

Gradient Descent $\mathcal{O}(IND)$

$$\text{Update rule: } \beta^{(k+1)} = \beta^{(k)} - \alpha \frac{\partial \mathcal{L}(\beta^{(k)})}{\partial \beta}$$

α is a parameter that needs to be chosen carefully.

The gradient for MSE comes out as:

$$\frac{\partial \mathcal{L}}{\partial \beta} = -\frac{1}{N} \tilde{\mathbf{X}}^T (\mathbf{y} - \tilde{\mathbf{X}}\beta)$$

Newton's method $\mathcal{O}(IND^2 + ID^3)$

It uses second order derivatives information to converge faster (we approximate the objective function by a quadratic function rather than a line).

$$\text{General rule: } \beta^{(k+1)} = \beta^{(k)} - \alpha \mathbf{H}_k^{-1} \frac{\partial \mathcal{L}(\beta^{(k)})}{\partial \beta}$$

where \mathbf{H}_k is the $D \times D$ Hessian at step k :

$$\mathbf{H}_k = \frac{\partial^2 \mathcal{L}(\beta^{(k)})}{\partial \beta^2}$$

Newton's method is equivalent to solving many least-squares problems.

Expectation-Maximization

EM is a family of methods to find a MLE/MAP estimator if some of the data is missing (e.g. latent variables):

Given is some data \mathbf{x} and a model with some latent variables \mathbf{z} and a likelihood $\mathcal{L}(\theta; \mathbf{x}, \mathbf{z})$ (e.g. a gaussian where we need to find the mean and the covariance). Goal is to find

$\beta = \arg \max_{\beta} \mathcal{L}_{lik}(\theta; \mathbf{x})$, i.e. the MLE given only the data, without knowing the latent variables.

The problem is, that this likelihood can oftentimes not be optimized in closed form with respect to θ .

The solution is EM: Iteratively find better θ , start with θ_0 and iterate with variable t :

- E-step calculates the \mathbb{E} of log likelihood, with respect to \mathbf{Z} given \mathbf{X} under the current estimate θ_t :
 $Q(\theta, \theta_t) = \mathbb{E}_{\mathbf{Z}|\mathbf{X}, \theta_t} [\log(p(\mathbf{X}, \mathbf{Z}|\theta)|X = \mathbf{x})]$
- M-step finds next estimate that maximizes:
 $\theta_{t+1} = \arg \max_{\theta} Q(\theta, \theta_t)$
- Iterate until convergence.

Regression

Simple linear regression: $y_n \approx \beta_0 + \beta_1 x_{n1}$

Multiple linear regression:

$$y_n \approx f(\mathbf{x}_n) := \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \dots + \beta_D x_{nD}$$

Linear basis function model

We can create more complex models while staying in the linear framework by transforming the inputs X of dimensionality D through a function $\phi: D \rightarrow M$.

$y_n = \beta_0 + \sum_{i=1}^M \beta_i \phi_i(\mathbf{x}_n) = \tilde{\boldsymbol{\phi}}^T(\mathbf{x}_n^T) \boldsymbol{\beta}$. The optimal $\boldsymbol{\beta}$ can be computed in closed form by $\boldsymbol{\beta} = (\tilde{\boldsymbol{\Phi}}^T \tilde{\boldsymbol{\Phi}})^{-1} \tilde{\boldsymbol{\Phi}}^T \mathbf{y}$ where $\tilde{\boldsymbol{\Phi}}$ is a matrix with N rows and the n -th row is $[1, \phi_1(\mathbf{x}_n), \dots, \phi_M(\mathbf{x}_n)]$.

But note this requires $\tilde{\boldsymbol{\Phi}}^T \tilde{\boldsymbol{\Phi}}$ to be invertible (well-conditioned: $\tilde{\boldsymbol{\Phi}}$ full column-rank).

$$\text{Ridge regression: } \boldsymbol{\beta}_{ridge} = (\tilde{\boldsymbol{\Phi}}^T \tilde{\boldsymbol{\Phi}} + \lambda \mathbf{I})^{-1} \tilde{\boldsymbol{\Phi}}^T \mathbf{y}$$

Cost functions

Cost function / Loss: $\mathcal{L}(\beta) = \mathcal{L}(\mathcal{D}, \beta)$

Mean square error (MSE): $\frac{1}{2N} \sum_{n=1}^N [y_n - f(\mathbf{x}_i)]^2$ convex, sensible to outliers

MSE matrix formulation: $\frac{1}{2N} (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$

Mean absolute error (MAE): $\frac{1}{2N} \sum_{n=1}^N |y_n - f(\mathbf{x}_i)|$ convex (not strict), not diff-able, reasonably robust

Huber loss: $\mathcal{L}_{\delta}(a) = \begin{cases} \frac{1}{2} a^2 & \text{for } |a| \leq \delta, \\ \delta(|a| - \frac{1}{2}\delta), & \text{otherwise.} \end{cases}$

same as MAE but diff-able

Root mean square error (RMSE): $\sqrt{2 * \text{MSE}}$

Epsilon insensitive ("hinge loss", used for SVM):

$$\mathcal{L}_{\epsilon}(y, \hat{y}) = \begin{cases} 0 & \text{if } |y - \hat{y}| \leq \epsilon, \\ |y - \hat{y}| - \epsilon, & \text{otherwise.} \end{cases}$$

Least squares $\mathcal{O}(ND^2 + D^3)$

Consistent, asymptotically normal.

The gradient of the MSE set to zero is called the normal equation: $-\mathbf{X}^T \mathbf{y} + \mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = 0$.

We can solve this for $\boldsymbol{\beta}$ directly (by matrix manipulation) $\boldsymbol{\beta} = (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T \mathbf{y}$

Classification

$$\text{Logistic Function: } \sigma(t) = \frac{\exp(t)}{1 + \exp(t)} = \frac{\exp(x)}{\exp(x) + 1}$$

$$\text{Derivative: } \frac{\partial \sigma(t)}{\partial t} = \sigma(t)[1 - \sigma(t)]$$

$$\text{Softmax function: } \sigma(\mathbf{z})_j = \frac{\exp(z_j)}{\sum_{k=1}^K \exp(z_k)}.$$

Classification with linear regression: Use $y = 0$ as class \mathcal{C}_1 and $y = 1$ as class \mathcal{C}_2 and then decide a newly estimated y belongs to \mathcal{C}_1 if $y < 0.5$.

Logistic Regression

$$\frac{\partial \mathcal{L}(\beta)}{\partial \beta} = \tilde{\mathbf{X}}^T [\sigma(\tilde{\mathbf{X}}\beta) - \mathbf{y}]$$

There's no closed form, we can use gradient descent.

Generalized linear model

The GLM consists of three elements:

- A probability distribution from the exponential family.
- A linear predictor $\hat{y} = \mathbf{X}\beta$.
- A link function g s.t. $E(y) = \mu = g^{-1}(\eta)$.

In a generalized linear model (GLM), each outcome of the dependent variables y is assumed to be generated from a particular distribution in the exponential family, a large range of probability distributions that includes the normal, binomial, Poisson and gamma distributions, among others.

Cost functions

$$\text{RMSE } \sqrt{\frac{1}{N} \sum_{n=1}^N [y_n - \hat{p}_n]^2}$$

$$\text{0-1 Loss } \frac{1}{N} \sum_{n=1}^N \delta(y_n, \hat{y}_n)$$

Log-Loss

$$-\frac{1}{N} \sum_{n=1}^N y_n \log(\hat{p}_n) + (1 - y_n) \log(1 - \hat{p}_n)$$

Probabilistic framework

The Likelihood Function maps the model parameters to the probability distribution of \mathbf{y} : $\mathcal{L}_{lik}: \text{parameter space} \rightarrow [0; 1] \quad \beta \mapsto p(\mathbf{y} | \beta)$ An underlying p is assumed before. If the observed y are IID, $p(\mathbf{y} | \beta) = \prod_n p(y_n | \beta)$.

\mathcal{L}_{lik} can be viewed as just another cost function.

Maximum likelihood then simply chooses the parameters β s.t. observed data is most likely.

$$\beta = \arg \max_{\text{all } \beta} L(\beta)$$

Assuming different p is basically what makes this so flexible. We can chose e.g.:

Gaussian p	$\mathcal{L}_{lik} \hat{=}$	$-\mathcal{L}_{MSE}$
Laplace p	$\mathcal{L}_{lik} \hat{=}$	$-\mathcal{L}_{MAE}$

It is a sample approximation of the expected likelihood: $\mathcal{L}_{lik}(\beta) \approx E_y[p(\mathbf{y} | \beta)]$

Bayesian methods

Bayes rule: $p(A, B) = p(A|B)p(B) = p(B|A)p(A)$

$$\underbrace{p(\mathbf{y}, \mathbf{z})}_{\text{joint}} = \underbrace{p(\mathbf{y}|\mathbf{z})}_{\text{likelihood}} \underbrace{p(\mathbf{z})}_{\text{prior}} = \underbrace{p(\mathbf{z}|\mathbf{y})}_{\text{posterior}} \underbrace{p(\mathbf{y})}_{\text{mar. li}}$$

Least-squares tries to find model parameters β which maximize the likelihood. Ridge regression maximizes the **posterior** $p(\beta|\mathbf{y})$.

Bayesian method are biased.

Bayesian networks

Variables \rightarrow observations

We can use a Directed Acyclic Graph (DAG) to define a joint distribution of events:

$$p(\mathbf{x}) = \prod_{k=1}^K p(x_k | \mathbb{P}_k)$$

We can then obtain the distribution over latent factors (z_i) by marginalizing over the unknown variables:

$$p(z_1, z_2, z_3 | y_1, y_2) = \frac{\text{joint}}{p(y_1, y_2)}$$

$$\Rightarrow p(z_1 | y_1, y_2) = \sum_{z_2, z_3} \frac{\text{joint}}{p(y_1, y_2)}$$

Sum-product

$$\sum_{z_3} \sum_{z_2} p(y_a | z_1, z_2) p(y_b | z_2, z_3) p(z_1) p(z_2) p(z_3) =$$

$$p(z_1) \sum_{z_2} p(y_a | z_1, z_2) p(z_2) \sum_{z_3} p(y_b | z_2, z_3) p(z_3)$$

Belief propagation

Belief propagation is a message-passing based algorithm used to compute desired marginals (e.g. $p(z_1|y_1, y_2)$) efficiently. It leverages the factorized expression of the joint. Messages passed:

$\mathbb{N}(i)$: set of all neighbours of i

$\mathbb{P}(a)$: set of all parents of a

variables to observations

$$m_{i \rightarrow a}(z_i) = p(z_i) \prod_{b \in \mathbb{N}(i) \setminus a} m_{b \rightarrow i}(z_i)$$

observations to variables $m_{a \rightarrow i}(z_i) =$

$$\sum_{z_j, \forall j \neq i} p(y_a | \mathbb{P}(a)) \prod_{k \in \mathbb{N}(a) \setminus i} m_{k \rightarrow a}(z_k)$$

Compute marginals by multiplying all the messages received at node i :

$$p(z_i | \mathbf{y}) = p(z_i) \prod_{a \in \mathbb{N}(i)} m_{a \rightarrow i}(z_i)$$

Kernel methods

Kernels are another way to encode our prior belief about the relation of outputs to inputs. A kernel defines a distance measure, or "similarity" of two vectors. We define:

$$(\mathbf{K})_{i,j} = \kappa(\mathbf{x}_i, \mathbf{x}_j) = \vec{\phi}(\mathbf{x}_i)^T \vec{\phi}(\mathbf{x}_j).$$

The ϕ are not that important in the end, because we only use the Kernel as is. Sometimes it's even impossible to write them down explicitly.

Linear	$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
Polynomial	$\kappa(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^T \mathbf{x}_j + c)^d$
RBF	$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\ \mathbf{x}_i - \mathbf{x}_j\ ^2}{2\sigma^2}\right)$

Properties of a Kernel:

- \mathbf{K} symmetric
- \mathbf{K} p.s.d. ($\mathbf{z}^T \mathbf{K} \mathbf{z} = \sum_i \sum_j K_{ij} z_i z_j$)

Gaussian Process $\mathcal{O}(N^3)$

The predicting function f is interpreted as a random variable with jointly gaussian prior: $\mathcal{N}(f | \mathbf{0}, \mathbf{K})$.

Defining the Kernel matrix $\mathbf{K} = \kappa(\mathbf{X}, \mathbf{X})$ defines the prior. The key idea is, that if \mathbf{x}_i and \mathbf{x}_j are deemed by the kernel to be similar, then we expect the output of f at those points to be similar, too.

We can sample functions from this random variable f and we can use prior + measurements to generate predictions.

If we have measurements \mathbf{y} available, we get a joint distribution with the $\hat{\mathbf{y}}$ to be predicted:

$$\begin{bmatrix} \mathbf{y} \\ \hat{\mathbf{y}} \end{bmatrix} = \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \kappa(\mathbf{X}, \mathbf{X}) + \sigma_n^2 \mathbf{I} & \kappa(\mathbf{X}, \hat{\mathbf{X}}) \\ \kappa(\hat{\mathbf{X}}, \mathbf{X}) & \kappa(\hat{\mathbf{X}}, \hat{\mathbf{X}}) \end{bmatrix}\right)$$

This can be conditioned on \mathbf{y} to find the PDF of $\hat{\mathbf{y}}$. Advantage: we output our prediction as probabilities (which represent uncertainty). Decrease variance by averaging.

Neural Networks

$\mathbf{x}_n \xrightarrow{\beta_i^{(1)}} a_i^{(1)} \xrightarrow{h} z_i^{(1)} \xrightarrow{\beta_i^{(2)}} \dots \xrightarrow{\beta_i^{(K)}} \hat{\mathbf{y}}_n$ A feed forward Neural Network is organized in K layers, each layer with $M^{(k)}$ hidden units $z_i^{(k)}$.

Optimization

- multiple start
- stochastic gradient

Backpropagation

It's an algorithm which computes the gradient of the cost \mathcal{L} w.r.t. the parameters $\beta^{(k)}$.

Forward pass: compute a_i , z_i and \mathbf{y}_n from \mathbf{x}_n .

Backward pass: work out derivatives from outputs to the target $\beta_i^{(k)}$. Using the chain rule:

$$\delta^{(k-1)} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{(k-1)}} = \text{diag}[h'(\mathbf{a}^{(k-1)})] \mathbf{B}^{(k)T} \delta^{(k)}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{B}^{(1)}} = \delta^{(1)} \mathbf{x}^T$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{B}^{(k)}} = \delta^{(k)} \mathbf{z}^{(k)T}$$

Regularization

NN are not *identifiable* (existence of many local optima), therefore the maximum likelihood estimator is not *consistent*.

NN are universal density estimators, and thus prone to severe overfitting. Techniques used to reduce overfitting include early stopping (stop optimizing when test error starts increasing) and "weight decay" (i.e. L_2 regularization).

Support Vector Machines

Search for the hyperplane separating the data s.t. the gap (margin) is biggest. It minimizes the following cost function ("hinge loss"):

$$\mathcal{L}_{SVM}(\beta) = \sum_{n=1}^N [1 - y_n \phi_n \beta]_+ + \frac{\lambda}{2} \sum_{j=1}^M \beta_j^2$$

with $[t]_+ = \max(0, t)$

This is convex but not differentiable. In the dual, the same problem can be formulated as:

$$\max_{\alpha \in [0; C]} \mathbf{N} \alpha^T \mathbf{1} - \frac{1}{2} \alpha^T \mathbf{Y} \mathbf{K} \mathbf{Y} \alpha, \quad \alpha^T \mathbf{y} = 0$$

Gaussian Mixture Models

In mixture models, the data is generated by a sum (a mix) of K models.

$$p(\mathbf{X} | \boldsymbol{\mu}, \boldsymbol{\Sigma}, \mathbf{r}) = \prod_{n=1}^N \prod_{k=1}^K \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{r_{nk}}$$

Marginal likelihood

$$p(\mathbf{x}_i | \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k p_k(\mathbf{x}_i | \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_i | \underbrace{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k}_{\boldsymbol{\theta}})$$

To use this for clustering, we first fit this mixture and then compute the posterior $p(z_i = k | \mathbf{x}_i, \boldsymbol{\theta})$. This yields *soft* cluster assignments.

Posterior distribution

$$p(z_i = k | \mathbf{x}_i, \boldsymbol{\theta}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

PCA $\mathcal{O}(M^2 D N + M^3 N + M^3 D)$

Lossy compression.

Find the eigenvectors of the covariance matrix $\mathbf{X}^T \mathbf{X}$ of the data. These form an orthonormal basis $\{\mathbf{w}_1, \dots, \mathbf{w}_N\}$ for the data in the directions that have highest variance. One can then use the first $L < D$ vectors to rebuild the data:

$$\hat{\mathbf{x}}_i = \mathbf{W} \mathbf{z}_i = \mathbf{W} \mathbf{W}^T \mathbf{x}_i, \text{ with } \mathbf{W} = [\mathbf{w}_1; \dots; \mathbf{w}_L].$$

This minimizes mean square error $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|^2$.

Alternating least squares:

$$\mathbf{Z}^T \leftarrow (\mathbf{W}^T \mathbf{W})^{-1} \mathbf{W}^T \mathbf{X}$$

$$\mathbf{W}^T \leftarrow (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{X}^T$$

SVD $\mathcal{O}(4D^2 N + 8DN^2 + 9D^3)$

Singular value decomposition

Exact factorization. $\mathbf{X} = \mathbf{U} \mathbf{S} \mathbf{V}^T$ where \mathbf{U} is $D \times N$, \mathbf{V} is $N \times N$ and \mathbf{S} is $N \times N$.

The singular values of a $N \times D$ matrix \mathbf{X} are the square roots of the eigenvalues of the $D \times D$ matrix $\mathbf{X}^T \mathbf{X}$

Low rank approximation

$$\tilde{\mathbf{X}} = \mathbf{W} \mathbf{Z}^T, \text{ where } \mathbf{W} = \mathbf{U} \mathbf{S}^{\frac{1}{2}}, \mathbf{Z} = \mathbf{V} \mathbf{S}^{\frac{1}{2}}$$

Clustering

K-means: Initialize $\mu_k \forall k$, then iterate:

1. For all n , compute r_n given μ .

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg \min_j \|\mathbf{x}_n - \mu_j\|^2 \\ 0 & \text{otherwise} \end{cases}$$

2. For all k , compute μ_k given r . $\mu_k = \frac{\sum_n r_{nk} \mathbf{x}_n}{\sum_n r_{nk}}$

Concepts

Convexity

f is called convex $f: \forall x_1, x_2 \in X, \forall t \in [0, 1]:$

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2).$$

Sum of two convex functions is convex.

Composition of a convex function with a convex, nondecreasing function is convex. Linear, exponential and $\log(\sum \exp)$ functions are convex.

Bias-Variance Decomposition

Bias-variance comes directly out of the test error:

$$\begin{aligned} \overline{teErr} &= E[(\text{observation} - \text{prediction})^2] = E[(y - \hat{y})^2] \\ &= E[(y - y_{true} + y_{true} - \hat{y})^2] \\ &= \underbrace{E[(y - y_{true})^2]}_{\text{var of measurement}} + E[(y_{true} - \hat{y})^2] \\ &= \sigma^2 + E[(y_{true} - E[\hat{y}] + E[\hat{y}] - \hat{y})^2] \\ &= \sigma^2 + \underbrace{E[(y_{true} - E[\hat{y}])^2]}_{\text{pred bias}^2} + \underbrace{E[(E[\hat{y}] - \hat{y})^2]}_{\text{pred variance}} \end{aligned}$$

	bias	variance
regularization	+	-
choose simpler model	+	-
more data	-	+
increase dimensionality	+	+

Identifiability

We say that a statistical model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ is identifiable if the mapping $\theta \mapsto P_\theta$ is one-to-one:

$$P_{\theta_1} = P_{\theta_2} \Rightarrow \theta_1 = \theta_2 \text{ for all } \theta_1, \theta_2 \in \Theta.$$

A non-identifiable model will typically have many local optima yielding the same cost, e.g.

$$\mathcal{L}(W, Z) = \mathcal{L}(aW, \frac{1}{a}Z)$$

Curse of dimensionality

With dimensionality increase, data point become arbitrarily far from each other. Or in other words, the volume of the space increases so fast that the available data become sparse.

Primal vs. Dual

Instead of working in the **column space** of our data, we can work in the **row space**:

$\hat{\mathbf{y}} = \mathbf{X} \boldsymbol{\beta} = \mathbf{X} \mathbf{X}^T \boldsymbol{\alpha} = \mathbf{K} \boldsymbol{\alpha}$, where $\boldsymbol{\beta} \in \mathbb{R}^D$ and $\boldsymbol{\alpha} \in \mathbb{R}^N$ and (like magic) \mathbf{K} shows up, the Kernel Matrix.

Representer Theorem: For any $\boldsymbol{\beta}$ minimizing $\min_{\boldsymbol{\beta}} \sum_{n=1}^N \mathcal{L}(y_n, \mathbf{x}_n^T \boldsymbol{\beta}) + \sum_{d=1}^D \lambda \beta_d^2$,

$$\exists \boldsymbol{\alpha} \text{ s.t. } \boldsymbol{\beta} = \mathbf{X}^T \boldsymbol{\alpha}.$$

When we have an explicit vector formulation of $\boldsymbol{\beta}$, we can use the matrix inversion lemma to get to the dual. E.g. for ridge regression:

$$\boldsymbol{\beta} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{X}^T \underbrace{(\mathbf{X} \mathbf{X}^T + \lambda \mathbf{I}_N)^{-1}}_{\boldsymbol{\alpha}} \mathbf{y}$$

In optimization, we get to the dual like this:

$$\begin{aligned} \min_{\boldsymbol{\beta}} g(\boldsymbol{\beta}) &\xrightarrow{1} \min_{\boldsymbol{\beta}} \max_{\boldsymbol{\alpha}} G(\boldsymbol{\beta}, \boldsymbol{\alpha}) \\ &\quad \downarrow 2 \\ \max_{\boldsymbol{\alpha}} g^*(\boldsymbol{\alpha}) &\xleftarrow{3} \max_{\boldsymbol{\alpha}} \underbrace{\min_{\boldsymbol{\beta}} G(\boldsymbol{\beta}, \boldsymbol{\alpha})}_{g^*(\boldsymbol{\alpha})} \end{aligned}$$

Consistency

An estimator is said to be consistent, if it eventually recovers the true parameters that generated the data as the sample size goes to infinity. Of course, this only makes sense if the data actually comes from the specified model, which is not usually the case. Nevertheless, it can be a useful theoretical property.

Efficiency

An estimator is called efficient if it achieves the Cramer-Rao lower bound: $\text{Var}(\boldsymbol{\beta}) \geq 1/I(\boldsymbol{\beta})$, where I is the Fisher information.

Reducing Overfitting

- penalize terms
- reduce dimensionality
- more data

Occam's Razor

It states that among competing hypotheses, the one with the fewest assumptions should be selected.

Random Forests

Randomize training data: Bagging

Randomize feature space: Randomized feature selection

Parameters: maximum tree depth, number of trees, value of m_{try} , sample size n' .

Credits

Most material was taken from the lecture notes of Prof. Emteyaz Khan.

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Source code available on : <https://github.com/zommerfelds/pcml-cheatsheet>