CPSC 540: Machine Learning

Density Estimation

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Supervised Learning vs. Structured Prediction

- In 340 we focused a lot on "classic" supervised learning:
  - Model $p(y \mid x)$ where y is a single discrete/continuous variable.
- In the next few classes we'll focus on density estimation:
  - Model $p(x)$ where x is a vector or general object.
- Structured prediction is the logical combination of these:
  - Model $p(y \mid x)$ where y is a vector or general object.
  - Can be viewed as "conditional" density estimation.

3 Classes of Structured Prediction Methods

3 main approaches to structured prediction:

1. Generative models use $p(y \mid x) \propto p(y, x)$ as in naive Bayes.
    - Turns structured prediction into density estimation.
        - But we'll want to go beyond naive Bayes.
    - Examples: Gaussian discriminant analysis, mixtures and Markov models, VAEs.

2. Discriminative models directly fit $p(y \mid x)$ as in logistic regression.
    - View structured prediction as conditional density estimation.
        - Lets you use complicated features x that make the task easier.
    - Examples: Conditional random fields, conditional RBMs, conditional neural fields.

3. Discriminant functions just try to map from x to y as in SVMs.
    - Now you don't even need to worry about calibrated probabilities.
    - Examples: Structured SVMs, fully-convolutional networks, RNNs.

Density Estimation

- The next topic we'll focus on is density estimation:

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \quad \tilde{X} = \begin{bmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \\ ? & ? & ? & ? \end{bmatrix}$$

  - What is probability of $[1\ 0\ 1\ 1]$?
  - Want to estimate probability of feature vectors x^i.

- For the training data this is easy:
  - Set $p(x^i)$ to "number of times x^i is in the training data" divided by n.

- We're interested in the probability of test data,
  - What is probability of seeing feature vector $\tilde{x}^i$ for a new example i.

Density Estimation Applications

- Density estimation could be called a "master problem" in machine learning.
  - Solving this problem lets you solve a lot of other problems.

- If you have $p(x^i)$ then:
  - Outliers could be cases where $p(x^i)$ is small.
  - Missing data in x^i can be "filled in" based on $p(x^i)$.
  - Vector quantization can be achieved by assigning shorter code to high $p(x^i)$ values.
  - Association rules can be computed from conditionals $p(x^i_j \mid x^i_k)$.

- We can also do density estimation on (x^i, y^i) jointly:
  - Supervised learning can be done by conditioning to give $p(y^i \mid x^i)$.
  - Feature relevance can be analyzed by looking at $p(x^i \mid y^i)$.

Unsupervised Learning

- Density estimation is an unsupervised learning method.
  - We only have x^i values, but no explicit target labels.
  - You want to do "something" with them.

- Some unsupervised learning tasks from CPSC 340 (depending on semester):
  - Clustering: what types of x^i are there?
  - Association rules: which x_j and x_k occur together?
  - Outlier detection: is this a "normal" x^i?
  - Latent-factors: what "parts" are x^i made from?
  - Data visualization: what do the high-dimensional x^i look like?
  - Ranking: which are the most important x^i?

- You can probably address all these if you can do density estimation.

Bernoulli Distribution on Binary Variables

- Let's start with the simplest case: $x^i \in \{0, 1\}$ (e.g., coin flips),

$$X = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

- For IID data the only choice is the Bernoulli distribution:

$$p(x^i = 1 \mid \theta) = \theta, \quad p(x^i = 0 \mid \theta) = 1 - \theta.$$

- We can write both cases

$$p(x^i \mid \theta) = \theta^{\mathcal{I}[x^i=1]}(1-\theta)^{\mathcal{I}[x^i=0]}, \text{ where } \mathcal{I}[y] = \begin{cases} 1 & \text{if } y \text{ is true} \\ 0 & \text{if } y \text{ is false} \end{cases}.$$

Maximum Likelihood with Bernoulli Distribution

- MLE for Bernoulli likelihood is

$$
\begin{aligned}
\underset{0\leq\theta\leq 1}{\operatorname{argmax}}\, p(X \mid \theta) &= \underset{0\leq\theta\leq 1}{\operatorname{argmax}} \prod_{i=1}^{n} p(x^i \mid \theta) \\
&= \underset{0\leq\theta\leq 1}{\operatorname{argmax}} \prod_{i=1}^{n} \theta^{\mathcal{I}[x^i=1]}(1-\theta)^{\mathcal{I}[x^i=0]} \\
&= \underset{0\leq\theta\leq 1}{\operatorname{argmax}} \; \underbrace{\theta^1\theta^1\cdots\theta^1}_{\text{number of } x_i = 1} \; \underbrace{(1-\theta)(1-\theta)\cdots(1-\theta)}_{\text{number of } x_i = 0} \\
&= \underset{0\leq\theta\leq 1}{\operatorname{argmax}}\, \theta^{n_1}(1-\theta)^{n_0},
\end{aligned}
$$

where n_1 is count of number of 1 values and n_0 is the number of 0 values.

- If you equate the derivative of the log-likelihood with zero, you get $\theta = \frac{n_1}{n_1+n_0}$.
- So if you toss a coin 50 times and it lands heads 24 times, your MLE is $24/50$.

Multinomial Distribution on Categorical Variables

- Consider the multi-category case: $x^i \in \{1, 2, 3, \ldots, k\}$ (e.g., rolling di),

$$X = \begin{bmatrix} 2 \\ 1 \\ 1 \\ 3 \\ 1 \\ 2 \end{bmatrix}.$$

- The categorical distribution is

$$p(x^i = c \mid \theta_1, \theta_2, \ldots, \theta_k) = \theta_c,$$

  where $\sum_{c=1}^{k} \theta_c = 1$.
- We can write this for a generic x as

$$p(x^i \mid \theta_1, \theta_2, \ldots, \theta_k) = \prod_{c=1}^{k} \theta_c^{\mathcal{I}[x^i = c]}.$$

Multinomial Distribution on Categorical Variables

- Using Lagrange multipliers (bonus) to handle constraints, the MLE is

$$\theta_c = \frac{n_c}{\sum_{c'} n_{c'}}. \quad (\text{“fraction of times you rolled a 4”})$$

- If we never see category 4 in the data, should we assume $\theta_4 = 0$?
  - If we assume $\theta_4 = 0$ and we have a 4 in test set, our test set likelihood is 0.
- To leave room for this possibility we often use “Laplace smoothing”,

$$\theta_c = \frac{n_c + 1}{\sum_{c'} (n_{c'} + 1)}.$$

- This is like adding a “fake” example to the training set for each class.

MAP Estimation with Bernoulli Distributions

- In the binary case, a generalization of Laplace smoothing is

$$\theta = \frac{n_1 + \alpha - 1}{(n_1 + \alpha - 1) + (n_0 + \beta - 1)},$$

- We get the MLE when $\alpha = \beta = 1$, and Laplace smoothing with $\alpha = \beta = 2$.
- This is a MAP estimate under a beta prior,

$$p(\theta \mid \alpha, \beta) = \frac{1}{B(\alpha, \beta)} \theta^{\alpha - 1}(1 - \theta)^{\beta - 1},$$

where the beta function B makes the probability integrate to one.

$$\text{We want } \int_\theta p(\theta \mid \alpha, \beta) d\theta = 1, \quad \text{so define} \quad B(\alpha, \beta) = \int_\theta \theta^{\alpha - 1}(1 - \theta)^{\beta - 1} d\theta.$$

- Note that $B(\alpha, \beta)$ is constant in terms of θ, it doesn't affect MAP estimate.

MAP Estimation with Categorical Distributions

- In the categorical case, a generalization of Laplace smoothing is

$$\theta_c = \frac{n_c + \alpha_c - 1}{\sum_{c'=1}^{k}(n_{c'} + \alpha_{c'} - 1)},$$

which is a MAP estimate under a Dirichlet prior,

$$p(\theta_1, \theta_2, \dots, \theta_k \mid \alpha_1, \alpha_2, \dots, \alpha_k) = \frac{1}{B(\alpha)} \prod_{c=1}^{k} \theta_c^{\alpha_c - 1},$$

where $B(\alpha)$ makes the multivariate distribution integrate to 1 over θ,

$$B(\alpha) = \int_{\theta_1} \int_{\theta_2} \cdots \int_{\theta_{k-1}} \int_{\theta_k} \prod_{c=1}^{k} \left[\theta_c^{\alpha_c - 1}\right] d\theta_k d\theta_{k-1} \cdots d\theta_2 d\theta_1.$$

- Because of MAP-regularization connection, Laplace smoothing is regularization.

General Discrete Distribution

- Now consider the case where $x^i \in \{0,1\}^d$ (e..g, words in e-mails):

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}.$$

- Now there are 2^d possible values of vector x^i.
  - Can't afford to even store a θ for each possible vector x^i.
  - With n training examples we see at most n unique x^i values.
  - But unless we have a small number of repeated x^i values, we'll hopelessly overfit.
- With finite dataset, we'll need to make assumptions...

Product of Independent Distributions

- A common assumption is that the variables are independent:

$$p(x_1^i, x_2^i, \dots, x_d^i \mid \Theta) = \prod_{j=1}^{d} p(x_j^i \mid \theta_j).$$

- Now we just need to model each column of X as its own dataset:

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix} \quad \rightarrow \quad X_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad X_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}, \quad X_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}.$$

- A big assumption, but now you can fit Bernoulli for each variable.
  - We used a similar independence assumption in CPSC 340 for naive Bayes.

Density Estimation and Fundamental Trade-off

- "Product of independent" distributions (with d parameters):
  - Easily estimate each θ_c but can't model many distributions.
- General discrete distribution (with 2^d parameters):
  - Hard to estimate 2^d parameters but can model any distribution.

- An unsupervised version of the fundamental trade-off:
  - Simple models often don't fit the data well but don't overfit much.
  - Complex models fit the data well but often overfit.

- We'll consider models that lie between these extremes:
  1. Mixture models.
  2. Markov models.
  3. Graphical models.
  4. Boltzmann machines.

Outline

Univariate Gaussian

- Consider the case of a continuous variable $x \in \mathbb{R}$:

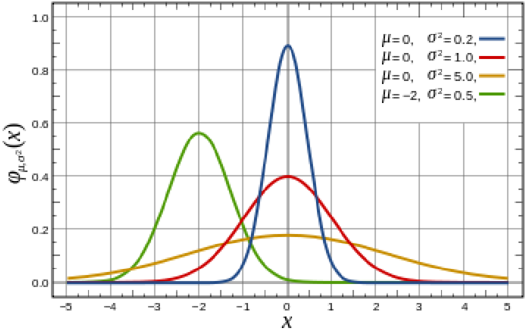
$$X = \begin{bmatrix} 0.53 \\ 1.83 \\ -2.26 \\ 0.86 \end{bmatrix}.$$

- Even with 1 variable there are many possible distributions.
- Most common is the Gaussian (or "normal") distribution:

$$p(x^i \mid \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x^i - \mu)^2}{2\sigma^2}\right) \quad \text{or} \quad x^i \sim \mathcal{N}(\mu, \sigma^2),$$

for $\mu \in R$ and $\sigma > 0$.

Univariate Gaussian



https://en.wikipedia.org/wiki/Gaussian_function

- Mean parameter μ controls location of center of density.
- Variance parameter σ^2 controls how spread out density is.

Univariate Gaussian

- Why use the Gaussian distribution?
  - Data might actually follow Gaussian.
    - Good justification if true, but usually false.
  - Central limit theorem: mean estimators converge in distribution to a Gaussian.
    - Bad justification: doesn't imply data distribution converges to Gaussian.
  - Distribution with maximum entropy that fits mean and variance of data (bonus).
    - "Makes the least assumptions" while matching first two moments of data.
    - But for complicated problems, just matching mean and variance isn't enough.
  - Closed-form maximum likelihood estimate (MLE).
    - MLE for the mean is the mean of the data ("sample mean" or "empirical mean").
    - MLE for the variance is the variance of the data ("sample variance").
    - "Fast and simple".

Univariate Gaussian (MLE for Mean)

- Gaussian likelihood for an example x^i is

$$p(x^i \mid \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x^i - \mu)^2}{2\sigma^2}\right).$$

- So the negative log-likelihood for n IID examples is

$$-\log p(X \mid \mu, \sigma^2) = -\sum_{i=1}^n \log p(x^i \mid \mu, \sigma^2) = \frac{1}{2\sigma^2}\sum_{i=1}^n (x^i - \mu)^2 + n\log(\sigma) + \text{const}.$$

- Setting derivative with respect to μ to 0 gives MLE of

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^n x^i. \quad (\text{for any } \sigma > 0),$$

so the MLE is the mean of the samples.

Univariate Gaussian (MLE for Variance)

- Gaussian likelihood for an example x^i is

$$p(x^i \mid \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x^i - \mu)^2}{2\sigma^2}\right).$$

- So the negative log-likelihood for n IID examples is

$$-\log p(X \mid \mu, \sigma^2) = -\sum_{i=1}^{n} \log p(x^i \mid \mu, \sigma^2) = \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x^i - \mu)^2 + n\log(\sigma) + \text{const.}$$

- Plugging in $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x^i$ and setting derivative with respect to σ to zero gives

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x^i - \hat{\mu})^2, \quad \text{(variance of the samples)}$$

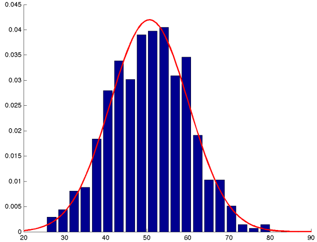
unless all x^i are equal (then NLL is not bounded below and MLE doesn't exist).

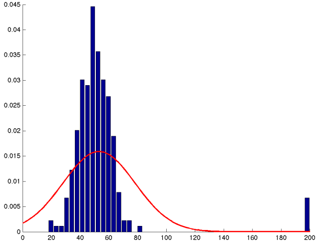
Alternatives to Univariate Gaussian

- Why not the Gaussian distribution?
  - Negative log-likelihood is a quadratic function of μ,

$$-\log p(X \mid \mu, \sigma^2) = \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x^i - \mu)^2 + n\log(\sigma) + \text{const.}$$

  so as with least squares the Gaussian is not robust to outliers.

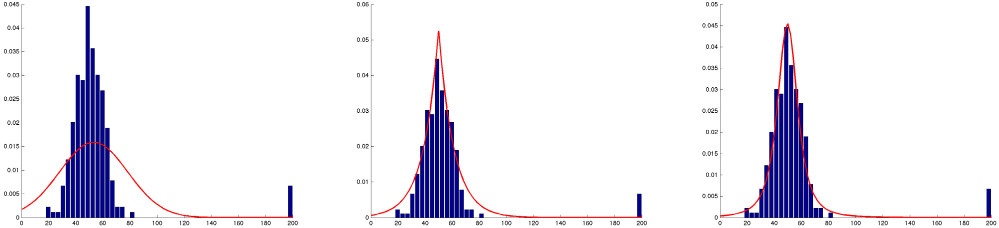




- This is a histogram of the x^i values, and the red line is the estimated density.
- We say Gaussian is "Light-tailed": assumes most data is close to mean.

Alternatives to Univariate Gaussian

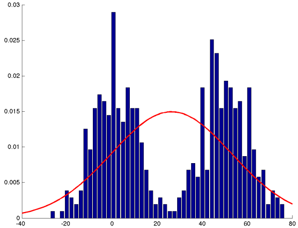
- Robust: Laplace distribution or student's t-distribution



- "Heavy-tailed": has non-trivial probability that data is far from mean.

Alternatives to Univariate Gaussian

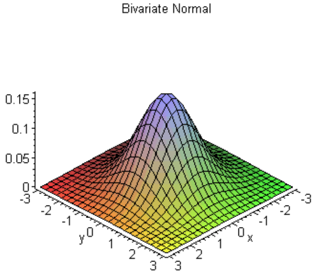
- Gaussian distribution is unimodal.



- Laplace and student t are also unimodal so don't fix this issue.
  - Next time we'll discuss "mixture models" that address this.

Multivariate Gaussian Distribution

- The generalization to multiple variables is the multivariate normal/Gaussian,



http://personal.kenyon.edu/hartlaub/MellonProject/Bivariate2.html

- We say that variables $x^i \in \mathbb{R}^d$ follow a multivariate Gaussian distribution if:
  - Linear combination $a^T x^i$ is a univariate Gaussian for any $a \in \mathbb{R}^d$.

Multivariate Gaussian Distribution

- The probability density for the multivariate Gaussian is given by

$$p(x^i|\mu,\Sigma) = \frac{1}{(2\pi)^{\frac{d}{2}}|\Sigma|^{\frac{1}{2}}}\exp\left(-\frac{1}{2}(x^i-\mu)^T\Sigma^{-1}(x^i-\mu)\right), \quad \text{or } x^i \sim \mathcal{N}(\mu,\Sigma),$$

  where $\mu \in \mathbb{R}^d$, $\Sigma \in \mathbb{R}^{d\times d}$ and $\Sigma \succ 0$, and $|\Sigma|$ is the determinant.

- Derived as an affine transformation of univariate standard normals (bonus).
  - Take $z_j^i \sim \mathcal{N}(0,1)$ and replace with $x^i = Az^i + \mu$ (where $\Sigma = AA^T$).

- If $|\Sigma| = 0$ we say the Gaussian is degenerate (bonus).
  - PDF does not integrate to 1 over all x^i.

Product of Independent Gaussians

- If we have d variables, we could make each follow an independent Gaussian,

$$x_j^i \sim \mathcal{N}(\mu_j, \sigma_j^2),$$

- In this case the joint density over all d variables is

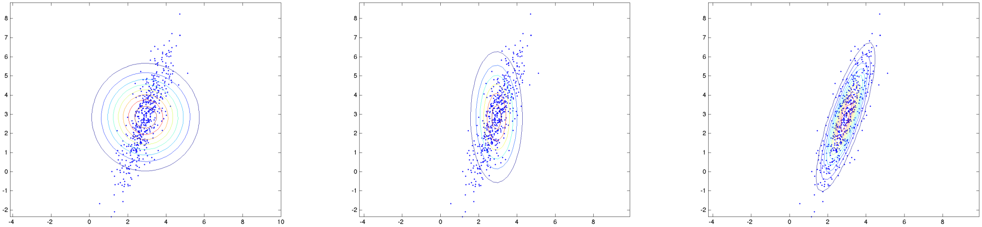
$$\begin{aligned}\prod_{j=1}^{d} p(x_j^i \mid \mu_j, \sigma_j^2) &\propto \prod_{j=1}^{d} \exp\left(-\frac{(x_j^i - \mu_j)^2}{2\sigma_j^2}\right) \\ &= \exp\left(-\frac{1}{2}\sum_{j=1}^{d} \frac{1}{\sigma_j^2}(x_j^i - \mu_j)^2\right) && (e^a e^b = e^{a+b}) \\ &= \exp\left(-\frac{1}{2}(x^i - \mu)^T \Sigma^{-1} (x - \mu)\right) && \text{(matrix notation)}\end{aligned}$$

where $\mu = (\mu_1, \mu_2, \dots, \mu_d)$ and Σ is a diagonal matrixwith diagonal elements σ_j^2.
- This is a special case of a multivariate Gaussian with a diagonal covariance Σ.

Product of Independent Gaussians

- The effect of a diagonal Σ on the multivariate Gaussian:
  - If $\Sigma = \alpha I$ the level curves are circles: 1 parameter.
  - If $\Sigma = D$ (diagonal) then axis-aligned ellipses: d parameters.
  - If Σ is dense they do not need to be axis-aligned: $d(d+1)/2$ parameters.

(by symmetry, we only need upper-triangular part of Σ)



- Diagonal Σ assumes features are independent, dense Σ models dependencies.

Summary

- Density estimation: unsupervised modelling of probability of feature vectors.
- Categorical distribution for modeling discrete data.
  - Beta and Diricihlet priors as priors that give closed-form MAP ("Laplace smoothing").
- Product of independent distributions is simple/crude density estimation method.
- Gaussian distribution is a common distribution with many nice properties.
  - Closed-form MLE.
  - But unimodal and not robust.
- Next time: going beyond Gaussians.

Lagrangian Function for Optimization with Equality Constraints

- Consider minimizing a differentiable f with linear equality constraints,

$$\underset{Aw=b}{\text{argmin}}\, f(w).$$

- The Lagrangian of this problem is defined by

$$L(w, v) = f(w) + v^T(Aw - b),$$

  for a vector $v \in \mathbb{R}^m$ (with A being m by d).
- At a solution of the problem we must have

$$\nabla_w L(w, v) = \nabla f(w) + A^T v = 0 \qquad \text{(gradient is orthogonal to constraints)}$$
$$\nabla_v L(w, v) = Aw - b = 0 \qquad \text{(constraints are satisfied)}$$

- So solution is stationary point of Lagrangian.

Lagrangian Function for Optimization with Equality Constraints

- Scans from Bertsekas discussing Lagrange multipliers (also see CPSC 406).

3.1 NECESSARY CONDITIONS FOR EQUALITY CONSTRAINTS

In this section we consider problems with equality constraints of the form

$$\begin{aligned} &\text{minimize} \quad f(x) \\ &\text{subject to} \quad h_i(x) = 0, \qquad i = 1, \ldots, m. \end{aligned} \tag{ECP}$$

We assume that $f : \Re^n \mapsto \Re$, $h_i : \Re^n \mapsto \Re$, $i = 1, \ldots, m$, are continuously differentiable functions. *All the necessary and the sufficient conditions of this chapter relating to a local minimum can also be shown to hold if f and h_i are defined and are continuously differentiable within just an open set containing the local minimum.* The proofs are essentially identical to those given here.

For notational convenience, we introduce the constraint function $h : \Re^n \mapsto \Re^m$, where

$$h = (h_1, \ldots, h_m).$$

We can then write the constraints in the more compact form

$$h(x) = 0. \tag{3.1}$$

Our basic Lagrange multiplier theorem states that for a given local minimum x^*, there exist scalars $\lambda_1, \ldots, \lambda_m$, called *Lagrange multipliers*, such that

$$\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(x^*) = 0. \tag{3.2}$$

There are two ways to interpret this equation:

(a) The cost gradient $\nabla f(x^*)$ belongs to the subspace spanned by the constraint gradients at x^*. The example of Fig. 3.1.1 illustrates this interpretation.

(b) The cost gradient $\nabla f(x^*)$ is orthogonal to the subspace of *first order feasible variations*

$$V(x^*) = \{\Delta x \mid \nabla h_i(x^*)'\Delta x = 0, \ i = 1, \ldots, m\}.$$

This is the subspace of variations Δx for which the vector $x = x^* + \Delta x$ satisfies the constraint $h(x) = 0$ up to first order. Thus, according to the Lagrange multiplier condition of Eq. (3.2), at the local minimum x^*, the first order cost variation $\nabla f(x^*)'\Delta x$ is zero for all variations

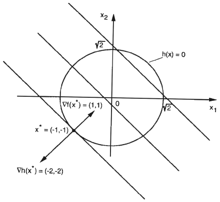


Figure 3.1.1. Illustration of the Lagrange multiplier condition (3.1) for the problem

$$\begin{aligned} &\text{minimize} \quad x_1 + x_2 \\ &\text{subject to} \quad x_1^2 + x_2^2 = 2. \end{aligned}$$

At the local minimum $x^* = (-1, -1)$, the cost gradient $\nabla f(x^*)$ is normal to the constraint surface and is therefore, collinear with the constraint gradient $\nabla h(x^*) = (-2, -2)$. The Lagrange multiplier is $\lambda = 1/2$.

Δx in this subspace. This statement is analogous to the "zero gradient condition" $\nabla f(x^*) = 0$ of unconstrained optimization.

Here is a formal statement of the main Lagrange multiplier theorem:

Proposition 3.1.1: (Lagrange Multiplier Theorem – Necessary Conditions) Let x^* be a local minimum of f subject to $h(x) = 0$, and assume that the constraint gradients $\nabla h_1(x^*), \ldots, \nabla h_m(x^*)$ are linearly independent. Then there exists a unique vector $\lambda^* = (\lambda_1^*, \ldots, \lambda_m^*)$, called a *Lagrange multiplier vector*, such that

$$\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla h_i(x^*) = 0. \tag{3.3}$$

If in addition f and h are twice continuously differentiable, we have

Lagrangian Function for Optimization with Equality Constraints

- We can use these optimality conditions,

$$\nabla_w L(w, v) = \nabla f(w) + A^T v = 0 \qquad \text{(gradient is orthogonal to constraints)}$$
$$\nabla_v L(w, v) = Aw - b = 0 \qquad \text{(constraints are satisfied)}$$

  to solve some constrained optimization problems.

- A typical approach might be:
  1. Solve for w in the equation $\nabla_w L(w, v) = 0$ to get $w = g(v)$ for some function g.
  2. Plug this $w = g(v)$ into the the equation $\nabla_v L(w, v) = 0$ to solve for v.
  3. Use this v in $g(v)$ to get the optimal w.

- But note that these are necessary conditions (may need to check it's a min).

MAP for Univariate Gaussian Mean

- Assume $x^i \sim \mathcal{N}(\mu, \sigma^2)$ and assume $\mu \sim \mathcal{N}(\mu_0, 1)$.
- The MAP estimate of μ under these assumptions can be written as

$$\hat{\mu} = \frac{n}{n+\sigma^2}\bar{x} + \frac{\sigma^2}{n+\sigma^2}\mu_0,$$

where $\bar{x}$ is the sample mean, $\frac{1}{n}\sum_{i=1}^n x^i$ (which is the MLE).

- The MAP estimate is a convex combination of the MLE and prior mean μ_0.
  - Regularizer moves us in a straight line away from MLE towards μ_0.

Maximum Entropy and Gaussian

- Consider trying to find the PDF $p(x)$ that
  1. Agrees with the sample mean and sample covariance of the data.
  2. Maximizes entropy subject to these constraints,

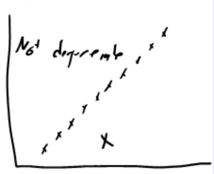
$$\max_p \left\{ - \int_{-\infty}^{\infty} p(x) \log p(x) dx \right\}, \quad \text{subject to } \mathbb{E}[x] = \mu, \ \mathbb{E}[(x-\mu)^2] = \sigma^2.$$

- Solution is the Gaussian with mean μ and variance σ^2.
  - Beyond fitting mean/variance, Gaussian makes fewest assumptions about the data.

- This is proved using the convex conjugate (see duality lecture).
  - Convex conjugate of Gaussian negative log-likelihood is entropy.
  - Same result holds in higher dimensions for multivariate Gaussian.

Degenerate Gaussians

- If $|\Sigma| = 0$, we say the Gaussian is degenerate.
- In this case the PDF only integrates to 1 along a subspace of the original space.
- With $d = 2$ degnerate Gaussians only have non-zero probability along a line (or just one point).



Multivariate Gaussian from Univariate Gaussians

- Consider a joint distribution that is the product univariate standard normals:

$$p(z^i) = \prod_{j=1}^{d} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(z_j^i)^2\right)$$
$$= \frac{1}{(2\pi)^{\frac{d}{2}}} \exp\left(\frac{1}{2}\langle z^i, z^i\rangle\right).$$

- Now define $x^i = Az^i + \mu$ for some (non-singular) matrix A and vector μ.
- The change of variables formula for multivariate probabilities is

$$p(x^i) = p(z^i)\left|\frac{\partial z^i}{\partial x^i}\right|.$$

- Plug in $z^i = A^{-1}(x^i - \mu)$ and $\frac{\partial z^i}{\partial x^i} = A^{-1}$...

Multivariate Gaussian from Univariate Gaussians

- This gives

$$p(x^i \mid \mu, A) = \frac{1}{(2\pi)^{\frac{d}{2}}} \exp\left(\frac{1}{2}\langle A^{-1}(x^i - \mu), A^{-1}(x^i\mu)\rangle\right) |\det(A^{-1})|$$
$$= \frac{1}{(2\pi)^{\frac{d}{2}} |\det(A)|} \exp\left(\frac{1}{2}(x^i - \mu)A^{-\top}A^{-1}(x^i - \mu)\right).$$

- Define $\Sigma = AA^\top$ (so $\Sigma^{-1} = A^{-\top}A^{-1}$ and $\det \Sigma = (\det A)^2$) to get

$$p(x^i \mid \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x^i - \mu)^\top \Sigma^{-1}(x^i - \mu)\right)$$

- So multivariate Gaussian is an affine transformtation of independent Gaussians.