Gradient Descent in Hilbert Space

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Outline

Banach Spaces

Definition

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Let X, Y be a normed vector spaces and $T : X \to Y$ a linear map. Then T is said to be **bounded** if there exists $C \geq 0$ such that for each $x \in X$,

$$\|Tx\| \leq C\|x\|$$

We define

$$L(X, Y) = \{T : X \to Y : T \text{ is linear and bounded}\}$$

Definition

Let $X_1, \ldots, X_n$ and Y be a normed vector spaces and $T : \prod_{j=1}^{n} X_j \to Y$ a multilinear linear map. Then T is said to be **bounded** if there exists $C \geq 0$ such that for each $(x_j)_{j=1}^{n} \in \prod_{j=1}^{n} X_j$,

$$\|T(x_1, \ldots, x_n)\| \leq C\|x_1\| \ldots \|x_n\|$$

We define

$$L^n(X_1, \ldots, X_n; Y) = \{T : X \to Y : T \text{ is multilinear and bounded}\}$$

If $X_1, \ldots, X_n = X$, we write $L^n(X, Y)$ in place of $L^n(X, \ldots, X; Y)$.

Remark

Let X and Y be normed vector spaces. We may identify $L(X, L(X, \dots, L(X, Y)) \dots)$ and $L^n(X, Y)$ via the isometric isomorphism given by $\phi \mapsto \psi_\phi$ where

$$\psi_\phi(x_1, x_2, \dots, x_n) = \phi(x_1)(x_2)\dots(x_n)$$

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Definition

Let X be a normed vector space over $\mathbb{R}$. We define the **dual space of** X, denoted X^*, by $X^* = L(X, \mathbb{R})$. Let $T : X \to \mathbb{R}$. Then T is said to be a **bounded linear functional on** X if $T \in X^*$.

Definition

Let X, Y be a banach spaces, $A \subset X$ open, $f : A \to Y$ and $x_0 \in A$. Then f is said to be **(1-st order) Frechet differentiable at** x_0 if there exists $Df(x_0) \in L(X, Y)$ such that,

$$f(x_0 + h) = f(x_0) + Df(x_0)(h) + o(\|h\|) \qquad \text{as } h \to 0$$

If f is Frechet differentiable at x_0, we define the **Frechet derivative of** f **at** x_0 to be $Df(x_0)$. We say that f is **(1-st order) Frechet differentiable** if for each $x_0 \in A$, f is Frechet differentiable at x_0.

If f is Frechet differentiable, we define the **Frechet derivative** of f, denoted $Df : A \to L(X, Y)$, by

$$x \mapsto Df(x)$$

Continuing inductively, if f is $(n-1)$-th order Frechet differentiable, f is said to be n-th order Frechet differentiable at x_0 if $D^{n-1}f$ is Frechet differentiable at x_0. We define $D^n f(x_0) = D(D^{n-1}f)(x_0)$.

Calculus

Remark

Note that $D^n f(x_0) \in L^n(X, Y)$.

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The tools used to obtain the following results:

- Frechet Derivative
- Bochner Integral
- Hahn-Banach Theorem

Result

Let X, Y be Banach spaces and $f \in L(X, Y)$. Then f is Frechet differentiable and for each $x_0 \in X$, $Df(x_0) = f$.

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Let X, Y, Z be Banach spaces, $f : X \to Y$, $g : Y \to Z$ and $x_0 \in X$. If f is Frechet differentiable at x_0 and g is Frechet differentiable at $f(x_0)$, then $g \circ f$ is Frechet differentiable at x_0 and

$$D(g \circ f)(x_0) = Dg(f(x_0)) \circ Df(x_0)$$

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Let X, Y be a Banach spaces, $A \subset X$ open and convex and $f : A \to Y$. If f is Frechet differentiable, then for each $x, y \in A$, there exists $t \in (0, 1)$ such that

$$\|f(x) - f(y)\| \leq \|Df(tx + (1 - t)y)\| \|x - y\|$$

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Let X, Y *be a Banach spaces,* $A \subset X$ *open and convex and* $f : A \to Y$*. Suppose that* f *is Frechet differentiable. If for each* $x \in A$*,* $Df(x) = 0$*, then* f *is constant.*

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Let X, Y be a Banach spaces, $A \subset X$ open and convex and $f, g : A \to Y$. Suppose that f and g are Frechet differentiable. If $Df = Dg$, then there exists $c \in Y$ such that $f = g + c$.

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Result

Let X *be a Banach spaces,* $A \subset X$ *open,* $f : A \to \mathbb{R}$ *and* $x_0 \in A$. *Suppose that* f *is Frechet differentiable at* x_0. *If* f *has a local minimum at* x_0, *then* $Df(x_0) = 0$.

Result

Let Y be a separable Banach space and $f \in C^1_Y(a, b)$. Then for each $x, x_0 \in (a, b)$, $x_0 < x$ implies that

1. *f' is Bochner integrable on $(x_0, x]$*
2. $$f(x) - f(x_0) = \int_{(x_0,x]} f' dm$$

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Let Y be a separable Banach space, $A \subset X$ open and convex, $f \in C^n_Y(A)$ and $x_0 \in A$. Then

$$f(x_0 + h) = \sum_{k=0}^{n} \frac{1}{k!} D^k f(x_0)(h, \dots, h) + o(\|h\|^n) \qquad \text{as } h \to 0$$

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Result

Let H be an inner product space. Then for each $x, y \in H$, $|\langle x, y \rangle| \leq \|x\|\|y\|$ with equality iff $x \in \mathrm{span}(y)$.

Definition

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Result

Let H be a Hilbert space. Then $\phi : H \to H^*$ defined above is an isometric isomorphism.

Definition

Let H be a Hilbert space, $f : H \to \mathbb{R}$ and $x_0 \in H$. Suppose that f is Frechet differentiable at x_0 so that $Df(x_0) \in H^*$. We define the **gradient of f at x_0**, denoted $\nabla f(x_0) \in H$, by

$$\nabla f(x_0) = \phi^{-1} Df(x_0)$$

That is, $\nabla f(x_0)$ is the unique element of H such that for each $y \in H$,

$$\langle \nabla f(x_0), y \rangle = Df(x_0)(y)$$

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Let H be a Hilbert space, $f : H \to \mathbb{R}$ and $x_0 \in H$. If f is Frechet differentiable at x_0, then

$$\operatorname*{arg\,min}_{\|h\| \leq 1} Df(x_0)(h) = -\|\nabla f(x_0)\|^{-1} \nabla f(x_0)$$

Remark

In the context of Hilbert spaces, the gradient allows us generalize the gradient descent method for minimization.

The idea is as follows. If $f : H \to \mathbb{R}$ is Frechet differentiable. Then

$$f(x_0 + h) \approx f(x_0) + \langle \nabla f(x_0), h \rangle$$

for h near 0. Taking $h = -\eta \nabla f(x_0)$ for some small $\eta > 0$ insures that h is close to 0 and h is in the direction of steepest descent of $Df(x_0)(v)$ which causes $f(x_0 + h) < f(x_0)$.

Convex Analysis

Result

Let X be a vector space, $A \subset X$ convex, $f : A \to \mathbb{R}$ convex and $x_0 \in A$. Then f has a local minimum at x_0 iff f has a global minimum at x_0.

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Result

Let X be a Banach space, $A \subset X$ open and convex, $f : A \to \mathbb{R}$ convex, $x_0 \in A$. Suppose that f is 2nd order Frechet differentiable. If for each $x_0 \in A$, $D^2 f(x_0) \in L^2(X, \mathbb{R})$ is positive semi definite (resp. pos. def.), then f is convex (resp. strictly convex).

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Remark

By positive definite, we mean $D^2 f(x_0)(h, h) > 0$ for $h \neq 0$.

Reproducing Kernel Hilbert Spaces

Definition

Let T be a set and $H \subset \mathbb{R}^T$ a hilbert space. For $t \in T$, we define the **evauluation functional at** t, denoted $L_t : H \to \mathbb{R}$, by

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If H is an RKHS, the Riesz representation theorem implies that for each $t \in T$, there exists $K_t \in H$ such that for each $f \in H$, $\langle K_t, f \rangle = f(t)$.

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If H is an RKHS, we define the **reproducing kernel** associated to H, denoted $K_H : T^2 \to \mathbb{R}$, by

$$K_H(s,t) = \langle K_s, K_t \rangle$$

Result

Let T be a set and $K : T^2 \to \mathbb{R}$. If K is symmetric and positive definite, then there exists a unique reproducing kernel Hilbert space $H \subset \mathbb{R}^T$ such that $K_H = K$.

Result

Let T be a set, $K : T^2 \to \mathbb{R}$ a symmetric, postivie definite kernel on T, $H \subset \mathbb{R}^T$ the corresponding RKHS, $t = (t_j)_{j=1}^n \subset T$ and $y = (y_j)_{j=1}^n \subset \mathbb{R}$.

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Define $L : H \to \mathbb{R}$ by

$$L(f) = \sum_{j=1}^{n} (y_j - f(t_j))^2 + \lambda \|f\|^2$$

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Put $\hat{f} = \arg\min_{f \in H} L(f)$.

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Then there exist $(\hat{\alpha}_j)_{j=1}^n \subset \mathbb{R}$ such that

$$\hat{f}(t) = \sum_{j=1}^{n} \hat{\alpha}_j K(t, t_j)$$

Remark

Define $A \in \mathbb{R}^{n \times n}$ by $A_{i,j} = K(t_i, t_j)$. Some regular calculus shows that $\hat{\alpha} = (A + \lambda I)^{-1} y$

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Question

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What if $(A + \lambda I)^{-1}$ is hard to compute?

Answer

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We can write rewrite $Q(f)$ as

$$Q(f) = \|L_t(f) - y\|_2^2$$

where $L_t \in L(H, \mathbb{R}^n)$ is given by

$$L_t(f) = (f(t_j))_{j=1}^{n}$$

Writing this out, we see that

$$\begin{aligned} Q(f_0 + h) &= \|L_t(f_0) - y\|_2^2 + 2(L_t(f_0) - y)^T L_t(h) + \|L_t(h)\|_2^2 \\ &= Q(f_0) + [\text{lin funct of } h] + [\text{bilin funct of } (h, h)] \end{aligned}$$

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Equating terms from Taylors theorem, we see that $D^2 Q(f_0)(h, h) = 2\|L_t(h)\|_2^2$, which is p.s.d. So Q is convex. Since norms are convex and $\lambda \geq 0$, L is convex.

Remark

Similar to before, writing out $L(f_0 + h)$, we get

$$L(f_0 + h) = L(f_0) + 2(L_t(f_0) - y)^T L_t(h) + 2\lambda\langle f_0, h\rangle + o(\|h\|^2)$$

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So

$$\begin{aligned} DL(f_0)(h) &= 2(L_t(f_0) - y)^T L_t(h) + 2\lambda\langle f_0, h\rangle \\ &= 2\sum_{j=1}^{n}(f_0(t_j) - y_j)\langle K_{t_j}, h\rangle + 2\lambda\langle f_0, h\rangle \\ &= \left\langle 2\left[\sum_{j=1}^{n}(f_0(t_j) - y_j)K_{t_j} + \lambda f_0\right], h\right\rangle \end{aligned}$$

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Hence

$$\nabla L(f_0) = 2\left[\sum_{j=1}^{n}(f_0(t_j) - y_j)K_{t_j} + \lambda f_0\right]$$

Remark

Therefore the gradient descent update reads as follows:

$$
\begin{aligned}
f_{t+1} &= f_t - \eta \nabla L(f_t) \\
&= (1 - 2\eta\lambda) f_t - 2\eta \left[\sum_{j=1}^{n} (f_0(t_j) - y_j) K_{t_j} \right]
\end{aligned}
$$

Applications to Gaussian Processes

Remark

Let T be a set and $x = (x_j)_{j=1}^n \in T^n$, $y = (y_j)_{j=1}^n \in \mathbb{R}^n$. Recall that if

$$\begin{aligned} y_i &= f(x_i) + \epsilon_i \\ \epsilon_i &\sim N(0, \sigma^2) \\ f &\sim GP(0, c) \end{aligned}$$

Then

$$f | x, y \sim GP(\tilde{\mu}, \tilde{c})$$

where

$$\tilde{\mu}(t) = c(t, x)[c(x, x) + \sigma^2 I]^{-1} y$$

and

$$\tilde{c}(s, t) = c(s, t) - c(s, x)[c(x, x) + \sigma^2 I]^{-1} c(x, t)$$

Remark

If $(c(x,x)+\sigma^2 I)^{-1}$ is too expensive to compute, we may set up the following convex optimization problems to approximate the posterior mean and posterior covariance functions via our gradient descent algorithm:

- $$\tilde{\mu}(t) = \arg\min_{f\in H} \sum_{j=1}^{n} (y_j - f(t_j))^2 + \sigma^2 \|h\|_H$$
- Fixing $t \in T$,
$$\hat{c}(\cdot, t) = \arg\min_{f\in H} \sum_{j=1}^{n} (c(x_j, t) - f(t_j))^2 + \sigma^2 \|h\|_H$$

where H is the RKHS corresponding to the p.d. kernel c.

Remark

The first optimization problem lets us approximate $\tilde{\mu}$ directly by gradient descent and the second optimization problem lets us approximate $\tilde{c}(t)$ by finding $\hat{c}(\cdot, t)$ via gradient descent and the computing $\tilde{c}(s,t) = c(s,t) - \hat{c}(s,t)$.

References

- analysis notes
- integration notes
- RKHS's
- Representer Theorem