Variational methods

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Today

- Revisiting Graphs, FEM, and GPs
- Final Projects
- No more exams, maybe 1 more HW

Variational Extensions

$$Av = b \iff \min_{v \in V} F(v)$$

Why is it desirable to reinterpret some of these methods as a variational problem?

1. Stability theory (graphs + FEM)
2. Flexibility
   ↳ add equality/inequality constraints to min problem (GPs)

③ Connection to physics

→ e.g. F is an energy

<u>ex 1</u> Graph Diffusion

$$\Delta_w u_i := \sum_{j \sim i} w_{ij} (u_j - u_i) = f_i$$

$$F[v] = \frac{1}{2} \sum_{i,j} w_{ij} (v_j - v_i)^2 - \sum_i f_i v_i$$

$$v \in V = \mathbb{R}^{N_{nodes}}$$

How are two connected?

Rewrite in vector/matrix notation

Recall $\delta v = v_j - v_i$

$$\delta^T F = \sum_{j \sim i} F_{ij}$$

Let $W = \mathrm{diag}(w_{ij}) \in \mathbb{R}^{N_{edges} \times N_{edges}}$

$$F[v] = \frac{1}{2} (\delta v)^T W \, \delta v - f^T v$$

$$= v^T \underbrace{\left(\frac{1}{2}\partial^T W \partial\right)}_{A} v - f^T v$$

To solve minimization problem

$$0 = \nabla_{v_k} F[\vec{v}] = \nabla_{v_k}\left(\sum_{i,j} v_i A_{ij} v_j - \sum_i v_i f_i\right)$$

$$= \left(\sum_{i,j} \delta_{ik} A_{ij} v_j + v_i A_{ij} \delta_{jk}\right) - v_k f_k$$

$$= \sum_j A_{kj} v_j + \sum_i v_i A_{ik} - v_k f_k$$

$$= (A + A^T) v - f$$

Noting $A = A^T$

$$2Av = f$$

$$\partial^T W \partial v = f$$

$$\sum_j w_{ij}(v_j - v_i) = f \qquad \text{At minimizer}$$

Now, let $u = \arg\min F(v)$

Now, let $u = \underset{v \in V}{\text{argmin}}\ F(v)$

$$\Rightarrow \quad F(u+\varepsilon v) \geq F(u) \quad \forall\, \varepsilon, v$$

and thus $\left.\frac{d}{d\varepsilon} F(u+\varepsilon v)\right|_{\varepsilon=0} = 0 \quad \forall v$

$$F(u+\varepsilon v) = \frac{1}{2} \sum_{ij} w_{ij} \left(u_j + \varepsilon v_j - u_i - \varepsilon v_i\right)^2 - \sum_i f_i (u_i + \varepsilon v_i)$$

$$= \frac{1}{2} \sum_{ij} w_{ij} \left[(u_j - u_i)^2 + \varepsilon (u_j - u_i)(v_j - v_i) + \varepsilon^2 (v_j - v_i)^2\right]$$
$$- \sum_i f_i u_i - \varepsilon \sum_i f_i v_i$$

$$\left.\frac{d}{d\varepsilon} F(u+\varepsilon v)\right|_{\varepsilon=0} = \frac{1}{2} \sum_{ij} w_{ij} (u_j - u_i)(v_j - v_i)$$
$$- \sum_i f_i v_i = 0$$

Variational Form of Graph Diffusion

Find $u \in V$ s.t. for any $v \in V$

$$a(u,v) = (v,f)$$
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$$(v,f) = \sum_i v_i f_i$$

$$(v,f) = \sum_i v_i f_i$$

$$V = \mathbb{R}^{N_{nodes}}$$

Remark: compare to FEM variational prob.

$$a(u,v) = \int \nabla u \cdot \nabla v \, dx$$
$$(v,f) = \int v f \, dx$$
$$V = H^1$$

Abstract Stability Analysis

i.e. cookbook for graphs & FEM

Recall Bilinear form $a(u,v)$ satisfies

$$a(\alpha u_1 + \beta u_2, v) = \alpha a(u_1, v) + \beta a(u_2, v)$$
$$a(u, \gamma v_1 + \delta v_2) = \gamma a(u, v_1) + \delta a(u, v_2)$$

Given energy $F(v) = a(v,v) - L(v)$

Let V be Hilbert space w/ inner product $(\cdot,\cdot)_V$ and norm $\|x\|_V = (x,x)_V$

Theorem Assume a, L satisfy

<u>Theorem</u> Assume a, L satisfy

1. <u>Symmetric</u> $a(u,v) = a(v,u)$
2. <u>Continuous</u> $|a(u,v)| < \gamma \|u\|_V \|v\|_V$

   for $\gamma > 0$ $\forall\, u,v \in V$

3. <u>V-elliptic</u> $a(v,v) \geq \alpha \|v\|_V^2$

   for $\alpha > 0$ $\forall\, v \in V$

4. <u>Continuous forcing</u> $|L(v)| \leq \Lambda \|v\|_V$

   for $\Lambda > 0$ $\forall\, v \in V$

then the solutions u

$$F(u) = \min_{v \in V} F(v) \quad \& \quad a(u,v) = L(v) \;\forall v \in V$$

are equivalent and have the stability result

$$\|u\|_V \leq \frac{\Lambda}{\alpha}$$

Why important → code won't blow up

→ uniqueness of exact sol

→ stability of discrete system

→ invertibility of discrete system

Pf – equivalence between energy min and variational problem exactly the same as the graph case we showed

– Take $v = u$ in variational prob

$$a(u,v) = L(v)$$

$$\alpha \|u\|_V^2 \le a(u,u) = L(u) \le \Lambda \|u\|_V$$

$$\alpha \|u\|_V \le \Lambda$$

$$\|u\|_V \le \frac{\Lambda}{\alpha}$$

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ex 2 Gaussian Processes & the "Optimal Recovery Problem"

Given a kernel $K : V \times V \to \mathbb{R}$

ex $K(x,y) = \exp\left(- \frac{\|x-y\|^2}{\ell^2}\right)$

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Define the "Reproducing Kernel Hilbert Space" aka RKHS space

$$\mathcal{H}_K = \text{span}\{K(x, x_i)\}_{i=1}^{N}$$

$\underline{ex}$ $f \in \mathcal{H}_K \Rightarrow f = \sum_i v_i \, K(x, x_i)$

Q? Define a kernel K so that

$\mathcal{H}_K = S$, our piecewise linear FEM space

Optimal Recovery Problem. Approx $Y \approx f(X) \in \mathcal{H}_K$

$$\min_{f \in \mathcal{H}_K} \|f\|_K^2 + \frac{1}{\varepsilon} \|f(x) - Y\|_0^2$$

$\underline{\text{Notation}} \rightarrow$ $f(x) = K(\cdot, x) \, V \leftarrow$ coefficients

$$\|f\|_K = f^T K^{-1} f$$

$$= v^T K K^{-1} K v$$

$$= v^T K v$$

Rewrite in terms of v

$$\min_{v \in \mathbb{R}^{N_n}} v^T K v + \frac{1}{\varepsilon} \|Kv - Y\|^2$$

Derivative wrt $v = 0$

$$0 = 2Kv + \frac{2}{\varepsilon} K^T (Kv - Y)$$

$$2Kv + \frac{2}{\varepsilon} K^T K v = \frac{2}{\varepsilon} KY$$

$$\varepsilon K v + K^T K v = KY$$

$$\varepsilon v + Kv = Y$$

$$(K + \varepsilon I) v = Y$$

$$v = (K + \varepsilon I)^{-1} Y$$

$$f = K(\cdot, x) v$$

$$= K(\cdot, x) (K + \varepsilon I)^{-1} Y$$

Exact same as $\mathbb{E}[Y | D]$ derived w/ Schur complement